CMFGEN MANUAL

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Introduction

CMFGEN: Radiative transfer code designed to solve the radiative transfer and statistical equilibrium equations in spherical geometry. It has been designed for applications to Wolf-Rayet (W-R) stars, O stars, Luminous Blue Variables (LBVs) and supernovae (SN). The mass-loss rate and velocity law must be specified --- at present we cannot solve for them self-consistently.

Three main modes are available:

Blanketing:
The effect of line overlap, and the effect of lines on the continuous energy distribution, is explicitly taken into account. It is the preferred mode that will give the most accurate results.

Sobolev:
Bound-bound transitions are treated using the Sobolev approximation. Good for fast-dirty models. Model is unblanketed, although collisional cooling is allowed for.

CMF:
Bound-bound transitions are computed as individual lines in the comoving-frame. **Obsolete, and may no longer work correctly.** Use Blanketing mode for accurate calculations, Sobolev mode for fast and crude calculations.

Several different options/assumptions are available to compute the radiation field. The normal default solves the static transfer equation for spherical geometry in the comoving-frame. Other options include (a) solving the static transfer equation in the plane parallel approximation with, or without, a velocity field, (b) solving the spherical transfer code allowing for relativistic terms, and (c) solving the time-dependent spherical transfer equation (still under development).

It is possible to treat species in different modes simultaneously. This is primarily useful for flux calculations (done with **CMF_FLUX**).

References

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Constraints on the Evolution of Massive Stars through Spectral Analysis. I. The WC5 Star HD165763.

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The treatment of non-LTE line blanketing in spherically expanding out flows.

Hillier, D.J. 1990, **A&A**, 231, 116.
An iterative method for the solution of the statistical and radiative equilibrium equations in expanding atmospheres.

Hillier, D.J. 1987, **ApJS**, 63, 947.
Modeling the extended atmospheres of WN stars

Program Names

cmfgen_dev.exe	Main program to compute atmospheric structure.
cmf_flux.exe	Compute observed spectrum.
dispgen.exe	General display package.
do_ng_v2.exe	Manual acceleration routine.
guess_dc.exe	Guess departure coefficients for a new model.
gramon_pgplot.f	General plotting package (called by other routines).
land_col_merge.exe	Merge two postscript files into a single file.
main_lte.exe	Compute Rosseland mean opacities.
n_col_merge.exe	Merge N postscript files into a single file.
rewrite_dc.exe	Rewrite departure coefficient file.
plt_jh.exe	Plot J, H etc from files with EDDFACTOR like formats.
plt_ip.exe	Plot/examine I as a function of impact parameter.
plt_spec.exe	Plot package to treat theoretical and observed spectra.
plt_scr.exe	Plot SCRTEMP file.
tlusty_vel.exe	Create a hydrostatic structure from a TLUSTY model.
wind_hyd.exe	Create a wind/theoretical hydrostatic structure.
wr_f_to_s.exe	Create/modify links between levels and super-levels

Species Names

Each atomic species has two abbreviations associated with it. These abbreviations are set in CMFGEN and MODEL_SPEC. The first abbreviation (e.g., CARB) refers to all ionization stages, and is used to set abundances etc. The second is used as the prefix for each ionization stage. At present the following abbreviations are in use. For consistency, and for the ease of moving models between users, it is best to stick with these definitions (or make minimal changes).

In this documentation, DUM is used to refer to the species (e.g., CARB) while XzV refers to a particular ionization stage (e.g., CIV).

Hydrogen	HYD	H
Helium	HE	He
Carbon	CARB	C
Oxygen	OXY	O
Nitrogen	NIT	N
Neon	NEON	Ne
Sodium	SOD	Na
Magnesium	MAG	Mg
Aluminum	ALUM	Al
Silicon	SIL	Sk
Phosphorous	PHOS	P
Sulfur	SUL	S
Argon	ARG	Ar
Calcium	CAL	Ca
Titanium	TIT	Tk
Vanadium	Van	V
Chromium	CHRO	Cr
Manganese	MAN	Mn
Iron	IRON	Fe
Cobalt	COB	Co
Nickel	NICK	Nk

Successive ionization stages are referred to as I, 2, III, IV, V, SIX, SEV, VIII, IX, and X. This mixed nomenclature was developed to facilitate code development, since it was easy to inadvertently write II instead of III etc. This is no longer of major concern, but has been left for consistency with earlier models.

Sk is used for Si (and Nk for Ni) since SiV could be interpreted as SIV. In a much older version we Sx for Si but there was still the possibility of confusion since SxI will conflict with SXI. The change over is transparent to new user, but users with very old files may need to modify VADAT, MODEL_SPEC, and batch.sh, files for consistency. Also note that SxIV_IN will become SkIV_IN. DISPGEN will still read old Silicon files in which case you should still use the Sx nomenclature for all options. A line in the new RVTJ files indicates the adopted convention.

Instead of using H, He etc. the abbreviations H_, He_ etc. could be used. This should cause no problems in CMFGEN, and would avoid any naming ambiguities and confusion. Unfortunately '_' is used in DISPGEN as species separator in DISPGEN commands. The separator could be changed in DISPGEN to something else (e.g., '-', '\', or '?'). Thus instead of

IF_ARG you would type IF-ARG
DC_Ar2 you would type DC-Ar_2

This does increase the amount of typing in DISPGEN. This approach could also be handled automatically, with a different convention string in RVTJ. Some minor editing of CMFGEN etc would be required. NB: DISPGEN is an integral part of CMFGEN and should be used as an examination tool.

The capitalization is important. While FORTRAN is generally case insensitive, string comparison commands are case sensitive. Thus FIX_HeI must be specified in the VADAT file, not FIX_HEI. Under VMS filenames are case insensitive. Unfortunately in UNIX file names are case sensitive. This can cause difficulties depending on how the files are opened.

Options in the display packages, **PLT_SPEC** and **DISPGEN**, are NOT case sensitive.

Program Units

For historical reasons the following units have been adopted:

Length Scales (e.g. R_*)	10^{10} cm
Opacity [CHI]	Chosen so that R. CHI is correct
Emissivity [ETA]	Chosen so that ETA/CHI is correct
Photoionization cross-sections:	Megabarns (in atomic data files only)
Densities	cm^{-3}
Temperature	10^4 K
Velocity	km s^{-1}
Mass	Solar mass: 1.989 10^{33} gm.
Luminosity	Solar luminosity: 3.826 10^{33} erg s^{-1}
Distances	kpc: 3.0856 10^{21} cm For PLT_SPEC the default distance is 1kpc.
Fluxes	Janskies - 1 Jy = 10^{-23} ergs/cm^2/sec/Hz In OBSFLUX, the fluxes assume d=1 kpc.
Physical constants	Function calls return cgs values.
Frequency	10^{15} Hz
Wavelengths	All plotting is done assuming vacuum wavelengths. Wavelength input can (generally) be for air (if λ > 2000 A) or for vacuum. In the atomic data files, wavelengths are generally air for λ > 2000 A; otherwise vacuum. Be careful --- there is the potential for confusion. In CMFGEN itself, only frequencies are used, so there is no confusion.
Adopted solar values:	R_{sun} = 6.96 10^{10} cm [6.95508 10^{10} cm] L_{sun} = 3.826 10^{33} erg s^{-1} [3.845 x 10^{33} cm] T_{eff}(sun) = 5784 K [5777K (5780) K] M_{sun} = 1.989 10^{33} gm. The values in brackets are from AAQ(2000). T_{eff} is only used for creating the MOD_SUM file. 5780 is calculated from R_{sun} and L_{sun}.
Abundances	Solar abundances are taken from Allen's Astrophysical Quantities by Cox (2000) p.29-31. For future reference, the adopted solar values are output to MOD_SUM.

Main Variables

Variable	Description	Typical Value
ND	Number of depth points	40 to 80
NC	Number of core rays	10 to 15
NP	Number of rays (angles)	ND+NC
NUM_BNDS	Number of bands used for linearization	3 (or 1 or 5)
NCF_MAX	Maximum umber of (continuum) frequencies	5,000 to 300,000
NLINE_MAX	Maximum number of lines in model	100,000
MAX_SIM	Number of bound-bound transitions that can be treated simultaneously	70 to 200
NXzV_F	Total number of levels in FULL ion XzV	Ion dependent
NXzV	Number of super levels for ion XzV	≤ NXzV_F
NXzV_IV	Number of important levels for ion XzV Only used in cmfgen_dev.exe	≤ NXzV
NT	Total number of unknown populations at each depth	100-2,000
NCF	Number of (continuum) frequencies	5,000 to 100,000

Notes:

1. The first 10 entries (9 for cmf_flux_v5.exe) are specified, in the MODEL_SPEC file, by the user.

2. NT is the total number of unknown populations at each depth. It is the sum of the NXzV + number of atomic species + 2 (for T and N_e)

3. The preferred value of NUM_BNDS is 3, which is a tradeoff between computational speed and memory. It (always) gives a good convergence with sufficient iterations, even without NG acceleration. NUM_BNDS=5 would reduce the total number of iterations (and possibly reduce execution time) but requires 50% more memory. It has not been full implemented in **CMFGEN_DEV.EXE**, as the BA matrix solver is not written).

   NUM_BNDS=1 is useful when running very large atomic models, since it requires a factor of 2 less memory than NUM_BNDS=3. In such cases it will also be faster per iteration. Unfortunately a given model will require (many) more iterations to converge, and overall the time needed to obtain a converged model will generally be longer. Further, the convergence is generally not as clear cut as with NUM_BNDS=3, and NG acceleration is an important tool for obtaining convergence.

4. ND is the number of depth points. In general 60 depth points is adequate for most models. **For dirty W-R** (and in many case more than adequate models) 40 depth points is satisfactory. The advantage of using a smaller ND is a smaller execution time, and less memory. In some cases convergence may be faster. **For O stars, at least** 60 depth points is HIGHLY recommended. Smaller values can lead to numerical instabilities, especially when using low turbulent velocities. Additional depth points (especially around the sonic point) may lead to improved convergence when numerical instabilities are occurring (e.g., persistent fluctuations in

the corrections at a single depth. The reason for the need for a higher number of points in O stars is that you need to have sufficient points in both the photosphere and the wind. Due to instabilities in the transfer equation it is not practical to have only a few points in the wind, even though its optical depth may be very small.

5. MAX_LINES should indicate the maximum number of lines that will be treated in the model. It is specified in MODEL_SPEC so that the necessary amount of memory can be allocated. If it is too small, an error message will be issued (to **OUTGEN**), and program execution will terminate.

6. NCF_MAX indicates the maximum number of continuum frequencies (which will also contain lines in BLANKETING mode) that will be treated in the model. It is specified in MODEL_SPEC so that the necessary amount of memory can be allocated. If it is too small, an error message will be issued (to **OUTGEN**), and program execution will terminate.

7. NCF is computed by CMFGEN. It is determined by the calculation mode (BLANK, SOB or CMF), and is dependent on VTURB, and the total number of bound-bound transitions in the model.

8. MAX_SIM should be large enough to handle the maximum number of lines whose intrinsic (i.e., Doppler) profiles overlap. For a large turbulent velocity, it may be necessary to increase its value. A very large value may slow down the linearization calculation as it partially determines how many lines influence the radiation field at the current frequency. Because of the velocity field, the radiation field at a given frequency can be influenced by lines at higher frequencies, even those outside the Doppler core. For H/He models MAX_SIM can be less than 20, while models with many iron-group elements it may need to be > 100. An error is output to OUTGEN if the value set in MODEL_SPEC is too small.

Versions

Only one version of CMFGEN is supplied. The executable is called

cmfgen_dev.exe

although this could easily be changed to cmfgen.exe by editing the Makefile in **dist/new_main**. An earlier version, **cmfgen.exe** is no longer supported, and is not supplied. The newer version should give very similar answers to the older version. To run the newer version of cmfgen, additional options will need to be set in VADAT. It is essential that users report any significant changes to John Hillier.

The primary difference with **cmfgen_dev.exe** is that the structure of the large variation matrix (BA) was altered in order to allow very large (& time consuming) models to be run.

CMFGEN_DEV.EXE uses an easily modified form of MODEL_SPEC. In this file, the number of "IMPORTANT LEVELS" is also specified. For H, CNO, and Fe these should be the same as the number of super-levels. For other elements they can often be be set to zero. The solution is not affected by the choice of IMPORTANT LEVELS --- only the rate of convergence. The optimal choice is not clear --- it is a tradeoff between memory and convergence. If some species give convergence difficulties, adjust the levels considered to be important. The inclusion of additional "IMORTANT LEVELS" increases the memory requirement but gives the faster convergence. We are still working on ways to improve convergence. **When all levels are regarded as IMPORTANT, the convergence is identical to cmfgen.exe**, while the memory requirement is slightly larger.

Memory

The main memory hog in CMFGEN is the BA matrix used to store the linearized statistical equations. In the worst case scenario, the amount of memory used by BA (and an associated matrix BA_PAR) is NT NT(NUM_BNDS+1)ND floating point words (typically 8 bytes on a workstation). For example, with NT=500, ND=60, and NUM_BNDS=3 at least 480 Megabytes of memory are required. When important levels are used, the memory is approximately NT NILV(NUM_BNDS+1)ND.

The BA array is accessed for every continuum frequency and for every line. To avoid excessive paging, it is **essential** that the BA matrix remain in memory. Thus the BA array limits the size of the atomic models. This memory limit is ultimately more important than execution time in determining the largest model that can be run.

A second substantial array is BAION (and BAION_PAR), which has dimensions NSPEC NT(NUM_BNDS+1)ND.

In the previous version of CMFGEN, BA is a 4 dimensional matrix with BA(I,J,K,L) giving the variation of the I^{th} statistical equilibrium equation at depth L with respect to species J at depth K. K only extends to NUM_BNDS, and is accessed such that 1 corresponds to L-1, 2 to L, and 3 to L+1.

In the current version the format of BA is different: SE(ID)%BA(I,J,K,L) where ID refers to the particular ionization stage, I refers to the statistical equilibrium equation for the ionization stage, J refers to the variation species but the numbering is dependent on ID. K and L have the same meaning as for the BA matrix. For convenience I will still refer to the variation matrix as the BA matrix in this document.

Execution Time

There is no simple formula that gives the execution time as a function of the fundamental variables. For smaller models, the execution time is proportional to NF ND^2. This scaling rises in the computation of the Eddington factors, and in the linearization. NF is the number of frequencies, and is roughly proportional to the number of lines (at least when not too large).

For models with many bound-bound transitions (e.g., > 30,000) other scalings may become important. For example, updating the BA matrix is proportional to NF NT ND. Due to excessive paging, models may grind to a halt if the BA array is too large to fit into physical memory.

The system dependent TUNE routine is supplied to determine in which routines or sections of the code most time is spent. On VMS systems the amount of paging is also output. TUNE statements already enclose most of the important sections of the code. NB. Due to excessive overheads, a call to TUNE should not be placed inside an innermost loop. It is worth checking the output of TUNE occasionally (as listed in the file TIMING) to verify that the timing of different code sections is not unusual; especially when moving to a new model regime, or a new computer.

NG acceleration

An option to perform an NG acceleration is supplied with the code. NG acceleration significantly improves convergence, particular when the corrections are small (e.g., < 10%). An NG acceleration can also be forced by hand using the stand-alone program DO_NG_V2, which reads, and updates, SCRTEMP.

It is recommended that NG accelerations only be performed when at least 15 (or more) iterations have been completed. This allows time for changes in the inner regions of the atmosphere to influence the outer regions. If applied too early, very large corrections, often of the wrong senses, may be predicted. I typically perform an NG acceleration when the corrections are less than 10%. In general the number of iterations is more important, than the size of the corrections. NG accelerations can be applied at each depth independently, over a range of depths, or to all depths at the same time. The later option is probably preferred when using a Diagonal operator, although in many cases I found that the applying the corrections to each depth independently was more efficient (particularly with Tri-diagonal error).

Even more sophisticated NG options could be envisaged. One difficulty is that in the early stages of a model, the nature of the iterations changes with iteration. For example, a FULL LINEARIZATION is usually followed by 1 or 2 Λ iterations. Further, the temperature in the outer regions of the stellar wind may be held fixed. This complicated iteration procedure has been adopted to ensure stable convergence.

As noted above, NG accelerations can be done outside the code execution by running DO_NG_V2. While having similar options to VADAT, it also has greater flexibility. In particular, the NG acceleration can be done using every n^{th} iteration, rather than consecutive can options. Further it is possible to simply average the last two iterations. After a manual NG acceleration, CMFGEN should be restarted.

Fixing the Linearization matrix (BA)

When the corrections to the populations are small the BA and BAION matrices do not need to be recomputed. They are thus saved, and read in when needed. This trick significantly reduces the computation time per iteration. The only drawback is that for large NT, a significant amount of disk space is needed.

I used to typically adopt 10% but have made changes to the code to allow more flexibility. The BA can be held fixed for several iterations, even when the corrections are very large. This can reduce the computation effort significantly. The optimal strategy is probably a function of the stellar parameters, and may also depend on the model initialization. NB: Lack of time, and continual changes to the models, has not allowed an optimal strategy, if it exists, to be determined. A similar statement also applies to NG acceleration.

Remember to delete the BAMAT and BAIONMAT files when a model is finalized (use the shell command clean (clean.sh) defined in aliases_for_cmfgen.sh. If using the developmental version, the ***SCRATCH*** files should also be deleted. These

*__SCRATCH*__ files allow more efficient solution of the simultaneous (rate) equations contained in the BA matrix, particularly when NT is large.

Convergence

CMFGEN defines an iteration as any cycle loop that changes the level populations. Thus the sequence

Λ-iteration,
full linearization,
full linearization,
full linearization,
full linearization,
NG Acceleration,
Λ-iteration,
full linearization,

constitutes 8 iterations. Other atmospheric codes might count this as only 5 iterations. The total number of iterations required to obtain a converged model depends on NUM_BNDS and, not surprisingly, on the parameters of the model. For the following discussion we assume NUM_BNDS=3.

The minimum number of iterations required for convergence is approximately 10. However, this only occurs when changing abundances of impurity species etc. A similar, or smaller number, may also be required if the number of super-levels associated with a given species is changed.

Generally 20 to 30 iterations are required, when using a tridiagonal operator, to obtain convergence of a NEW model (i.e., a model with new stellar parameters) to 0.1%. The convergence refers to the MAXIMUM correction obtained on the last iteration. The actual convergence achieved depends on depth, and the level under consideration. Usually the corrections to a given population form a geometric series: Thus if

r = (previous correction)/(current correction) = b/a

an estimate of the true error is $\mathbf{a/r + a/r^2 + a/r^3}$ ... which is approximately $\mathbf{a/(r-1)}$. In general, r is only slightly larger than unity. In practice, this error is too pessimistic if calculated using the maximum error returned in OUTGEN. Usually the maximum error is for an unimportant level at an unimportant depth. When successive corrections are less than 0.1%, the observed spectrum usually shows negligible changes between successive iterations. When using the tridiagonal operator, it is relatively easy (but not warranted) to improve the model convergence to less than 0.0001%.

For some models 60, or more, iterations may be required. The need for this many iterations can occur in several ways:

- The atmosphere is intrinsically unstable. Small changes in the stellar parameters result in large changes in the populations at some depths. In this case little can be done to improve convergence.
- An ionization front (discontinuity) has formed in the wind. CMFGEN is trying to eat its way through. Fudging the populations by hand can often assist in obtaining convergence.
- A few levels at one depth (or a few depths) have very bad population estimates. Successive iterations don't appear to be changing the estimates. When the populations are examined, they are found to be anomalous with respect to those at surrounding depths. Fudging the populations by hand will assist in obtaining convergence. Including additional depth points at the region of instability may also improve convergence.

```
You are using cmfgen_dev.exe with levels omitted from the full
      linearization. Inclusion of additional levels (usually for the most
      abundant species) will help convergence.
You are using a diagonal operator, which has an inherently slower
      asymptotic convergence than the tridiagonal operator.
```

Features and Bugs

CMFGEN is a large complicated program. As such it will contain bugs. The VADAT file contains over 100 options --- it is **IMPOSSIBLE** to test each option every time the code is updated. Obsolete options, or those not used very much, are more likely to cause problems. **PLEASE CHECK YOUR CALCULATIONS FOR UNEXPECTED RESULTS.** Many (too many!) diagnostic files are created to ensure that your results are reasonable.

Please report all bugs, no matter how trivial, immediately. We are working on a WEB page where these bugs can be reported and checked.

Extensive comparisons have been made, and are being made, with TLUSTY (the plane parallel code created by Hubeny and Lanz). In general there is excellent agreement. We are working on eliminating the SMALL discrepancies.

Known features:

When using the CMF option, NP must be ND+NC-2, otherwise it should be ND+NC.

Clumping has only been fully implemented in BLANKETING mode. In SOBOLEV mode, the correct EWs are computed, but the variation routine still needs to be fixed. This will be fixed SOMETIME in the near future.

When T is adjusted in an input file, the departure coefficients should also be adjusted. This is not trivial. It would probably be better to read in the populations in the outer layers, but we are unable to do this at present. An option in DISPGEN can be used.

The **CMF_FLUX** calculation may crash (although this is now very rare using the **[FRM_OPT]=INT** option) with a floating point overflow exception. If the error occurs try changing LAMBDA_ITERATION in CMF_FLUX_SUB_V5 to .FALSE., and recompile/link CMF_FLUX. As a consequence of the change, CMF_FOR_SOL_V2 will not be called.

Atomic data bug:

One of the lower levels in the NI data has the wrong statistical weight. I will fix this soon as I get a chance. It's not a simple change, since the f values to the state may change (depending on where they come from etc).

Some line wavelengths are not accurate. These will be fixed as they become known, and when I find time.

Installation

For installation purposes it is recommended that you adopt the same directory structure outlined below. This will automatically be obtained when you un-tar the distribution package.

Routines required by CMFGEN:

PGPLOT	Free package available off the WEB. Used for line drawings.
BLAS	Basic procedures for performing matrix manipulations. Should be available with the F90 compiler. If not, generic FORTRAN routines are supplied, **but these will be less efficient** than the system dependent BLAS routines.
LAPACK	FORTRAN numerical library. Often comes with F90 compiler. If not, routines available on the WEB. Several are supplied.

All atomic data should be stored in directories of the form

    something/ATOMIC/DUM/XzV/date

where date is of the form ddmmyy. This storage method will facilitate updates, bookeeping, and transfer of files to collaborators. Several different data sets already exist for some species. **Its a nightmare. NB.** For the atomic data directories, we tend to use, I, II, III, IV etc instead of the usual CMFGEN conventions.

It is suggested that you locate **cmfgen** in a distribution directory of the form

    cmfgen/27apr00/

In the following this distribution directory will be referred to as **dist/.**

Makefile

The distribution comes with Makefiles which will allow compilation of CMFGEN on your UNIX system. To avoid problems/inconsistencies use **GNU make**. To use these Makefiles do the following:

Edit Makefile_definitions in the **dist/** directory. Change it to ensure the following:

1. The distribution directory is defined.
2. It uses your f90 compiler.
3. The correct f90 flags have been set.
4. The library locations are correct.

Then

`make clean` — Removes all object files, libraries, executables from the distribution directories

`make -i >& HOPE` — Do the compilation. All error messages will be output to the file HOPE. -i indicates to ignore any warning messages which may be necessary on some systems. **Try to avoid the -i option, if possible.** If the compilation/linking works, the directory dist/exe will contain the following:

cmf_flux.exe	do_ng.exe
cmfgen.exe	append_dc.exe
dispgen.exe	rewrite_dc.exe
plt_spec.exe	plt_jh.exe
plt_jh.exe	wr_f_to_s.exe

If there is a failure, individual Makefiles in the sub-directories can be executed simply by typing

```
make
```

in the relevant sub-directory.

Makefile System Dependencies

Redhat 6.1	Supplied Makefiles work moderately well, with only a few minor (and insignificant) problems.
DEC OSF Alpha	Makefiles supplied with package may cause problems unless GNU make is used. Those in linux_make.tar (which contains only Makefiles) will work with the OSF make, although not perfectly. These have minor modifications from those supplied with the general distribution, and will allow the full installation to proceed. Some of the Makes seem to have features which don't work properly (e.g. library dependencies). These Makefiles can be installed using the command tar -xvf linux_make.tar in the installation directory. If you improve these files, please make a new linux_make.tar so I can distribute it. To make this file do the following (in **/dist**): set MAKELIST=`find . -name Makefile\*` tar cvf linux_make.tar $MAKELIST
HP Unix	Problems --- not yet done.

Possible Compilation Problems

1. The programs are written in f90 fixed format style. Most compilers can figure this out for themselves, but some need help. It may depend on the extension.

2. Several programs (e.g., CMFGEN, CMF_FLUX, DISPGEN) use modules for data storage. In these modules, data types are defined. For example, **mod_cmfgen.f**, defines the data type MODEL_ATOM_DATA. In f90, all arrays in these data types must be declared as a POINTER. This is **VERY** inefficient. The new standard now allows arrays to be declared ALLOCATABLE. Some of the new modules have been converted to use ALLOCATABLE arrays, but these may not compile with older compilers. If this is the case convert to the POINTER approach. Note that the behaviour and structure of CMFGEN and its routines is independent of which declaration is used.

3. For historical reasons most routines use the notation:
   REAL*8
   Most compilers have switches to change/overed this. On alphas, with the FUJI compiler and with the INTEL compiler, these definitions are fine. If not, it is relatively easy to use the SED editor to change all occurrences of REAL*8 to REAL. Hopefully, all routines just use INTEGER for integer declarations. NB: It is important that INTEGER and INTEGER*4 refer to the same sized variable.

   The supplied BLAS routines use DOUBLE_PRECISION notation.

   All programs use REAL*8 with one exception (discussed below).
   All programs can be compiled to use the default INTEGER size.

   The only routine that uses REAL*4 is the data storage module (MOD_CURVE_DATA) for GRAMON_PGPLOT, which is used to store the PLOTS. This is done simply to conserve memory. Data to GRAMON_PGPLOT is generally passed as REAL*8. A few routines routines don't use the REAL*8 notation, but this should be taken care of in the MAKKEFILE.

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4. Some compliers may insist on certain file extensions. A HP compiler will not compile programs of the form *.for.

5. Some routines will give compilation warnings. They should have no effect. Typical warning messages are:
   Passed variables not used in subroutine.
   Variable defined but not used.
   Variable set but not used.
   While some of these could be fixed it might necessitate a change in the calling routine etc. Some are given for FORTRAN parameters which I nearly always define, but which may not be used in the particular routine under consideration.

6. On some compilers \ is interpreted as a control character. For reasons known to no one I use this character in the atomic data files as a delimiter. Thus you may need a switch on the compiler to ensure that \ is not interpreted as a control character.

There may be a few compiler dependent features. For example, some compilers insist on writing 1X in format statements (instead of just X). I fixed as many as I know about but…

7. Under DEC OSF on an ALPHA, record alignment problems may be encountered. I have no idea what causes these, nor a general prescription for their removal. The last time this problem occurred it was solved (temporarily?) by moving the declaration

   TYPE(MODEL_ATOM) ATM()

   to the end of the module declaration file. None of the compiler options appeared to make a difference.

8. On pentium machines using LINUX, the INTEL Complier 60 IFC F90 code contained several bugs which affects the compilation of CMFGEN. The compiler also uses work.pc and work.pcl files. As a consequence the supplied makefiles do not work. A list of known bugs, and how to create the work.pcl files, can be supplied if needed.

9. The **INTEL Compiler 70 IFC F90** generally works much better than the earlier versions. As yet, I have not the latest modified relrase (version 8) on Pentium systems. The Makefiles, as supplied with the distribution, work with Redhat Linux 7.3. The appropriate compilation flags for the IFC compiler are given in **Makefile_definitions**. For the compilation to additional steps need to be done.

   a. Copy $cmfdist/unix/tune_intel.f $cmfdist/unix/tune.f
   b. Copy $cmfdist/new_mainmod_subs//mod_cmfgen_intel.f
      $cmfdist/new_main/mod_subs/mod_cmfgen.f (see 2 above)

Directory Structure

It is **STRONGLY** suggested that the same directory structure be retained when copying the code. This will make upgrades easier. On UNIX systems, the FORTRAN files are generally lower case, and are given the extension '.f' rather than '.FOR'. Since FORTRAN is NOT case sensitive, the '*.INC' files MUST be upper case (generally).

Current model is stored in **dist/**…

main/ No longer used.

new_main/ Main program and Fortran "include" files for main program. Some INC files have been converted to subroutines.

```
cmfgen.for              !Main Calling routine
cmfgen_sub.for          !Workhorse
GET_J_CHI.INC
```

There also several sub-directories with routine specific to this version.

new_main/mod_subs/ Contains module definitions for use with cmfgen. At present two versions of mod_cmfgen.f are suppied. The default uses the new fortran structure which allows allocatable arrays to be used in structures. Some compiler versions (e.g., INTEL) do not yet allow this option, so use mod_cmfgen.f_intel. No other changes to the code are required.

new_main/subs New subroutines. Kept in this locoation for simplicity.

com/ Contains simple scripts to facilitate running models etc.

disp/ Contains DISPGEN display package.

misc/ Collection of routines useful for a variety of purposes including generating atomic data, operating on departure coefficient files and generating F_TO_S link files.

newsubs/ Some new routines that replace routines in subs/. Primarily to do with the new version which uses dynamic memory allocation and records for the atomic populations. Kept here for convenience. The names are distinct.

obs/ Routines CMF_FLUX and OBS_FRAME used for computing the observed spectrum. CMF_FLUX is the main routine: OBS_FRAME is primarily used for testing, and requires J, χ, and η output from CMF_FLUX.

pgplt/ Plotting packages for DISPGEN and PLT_SPEC. These routines utilize PGPLOT, which is freely available and runs on many different platforms.

palne/	Contains subroutines for undertaking radiative transfer in plane-parallel geometry. Relativistic radiative transfer routines are also located in this directory.
spec_plt/	Contains PLT_SPEC package for displaying theoretical and model spectra.
subs/	Main directory with most of the subroutines required by CMFGEN.
tools/	Directory containing useful tools such as GEN_IN and USR_OPTION
unix/	A few routines (e.g., tune.f) that may be system dependent.

Useful Scripts

Several useful scripts are obtained in the [.COM] (i.e. /com) directory. To use these scripts:

Edit the file /com/aliases_for_cmfgen.sh. Replace all occurrences of ~hillier by the directory containing CMFGEN (e.g., /CMFGEN/30JUN00). In some of the scripts you may need to change the source locations of the **csh**, **tcsh** and **perl**.

Put the command

```
source /dist/com/aliases_for_cmfgen.sh
```

Source the file. This will define the following commands:

clean	Cleans model directory after model completion. Removes unwanted files such as EDDFACTOR, BAMAT, BAION etc. Only use the command after you're satisfied with the convergence of the model. To recover these files you will need to do a single iteration.
rmlinks	Removes soft links. This option was improved so that it only removes links in the current directory, and it shows what it is doing.
rm_all_links	Removes soft links, in the current directory, and all lower directories.
rmin	Removes all files of the form *_IN (no prompt)
rmrrr	Removes all files of the form *PRRR (prompt)
astxt	Creates soft links to the help files required by DISPGEN, PLT_SPEC, and WR_F_TO_S.
out2in	Renames all files of the form *OUT to *_IN
inc2inc	Renames files of the form abcde.inc to ABCDE.INC
fortof	Renames files of the form abcde.for to abcde.f
full_diff	Compiles ALL *.f, *.sh, *.INC and Makefile files in one directory with those in another. If only one directory is supplied as an parameter, the current directory is assumed to be the primary directory
for_diff	Compiles ALL *.f files in one directory with those in another. If only directory is supplied as an parameter, the current directory is assumed to be the primary directory
INC_diff	Compiles ALL *.INC files in one directory with those in another. If only directory is supplied as a parameter, the current directory is assumed to be the primary directory.

If you have alternative and better methods let me know.

Model computation

There are 4 primary control files:

batch.sh	Controls model execution, and creates soft links to the atomic data .
MODEL_SPEC	Specifies atomic models, number of depth points etc.
VADAT	Principal control which is used to describe the model, and assumptions used for its computation.
IN_ITS	Contains the maximum number of iterations to be attempted, and can also be used to force Lambda iterations.

These are described more fully elsewhere. Many other data files are also needed.

To generate a new model it is easiest to use the output from a previously converged model. This model should have parameters close to the new model (e.g. a factor of 2 in mass-loss rate). Exactly how close depends on the parameter regime. Some models will converge for much larger parameter changes. To initiate a model copy all the required input data files (discussed below) to the directory of the new model, as shown below.

```
cp r1/*OUT        r2/
cp r1/VADAT       r2/
cp r1/batch.sh    r2/
cp r1/MODEL_SPEC  r2/
cp r1/IN_ITS      r2/
cp r1/GAMMAS      r2/GAMMAS_IN
```

In the above **r1** is the old model directory and **r2** is the new model directory

Change the *OUT files to *_IN by typing

```
out2in
```

A simple script, cpmod, has been created to do the above. Simply type

```
cpmod r1 r2
```

In general, running a model requires the following steps to be performed.

Edit the **MODEL_SPEC** file so that the correct species and ionization stages are specified. Set the number of depth points, core rays, and impact-rays for the model. When running sequences of models, such changes will be minimal. Make sure that you have a XzV_IN file for all ionization stages if running a new model. NB: For an existing model, the populations will be obtained from SCRTEMP --- you do not need to change the XzV_IN files.

Edit the **batch.sh** file so it points to the appropriate directory. On VMS systems, use DEFINE (or ASSIGN) to link the atomic data files. On a Unix system, soft-links can be used.

Edit the **VADAT** file to set the parameters of the NEW model. If it is truly a new model, with new stellar parameters, set **[LIN_INT]** to F. If you are testing the influence of the number of grid points, or the effects of different SL assignments, etc, set **[LIN_INT]** to T (see description of VADAT options).

NB: If ArIII has been deleted from the MODEL_SPEC file, it is no longer necessary to delete all occurrences of ArIII (e.g. FIX_ARIII) from the VADAT file.

Edit the **IN_ITS** file to give the required number of iterations, typically 60. A model will terminate when it has converged (with the convergence requirement specified in **VADAT**) or after the specified number of iterations.

Finally, type **batch.sh &** to start the model. If the file crashes, check **OUTGEN** and **batch.log**. If the model does not converge in the number of iterations allocated (in IN_ITS), but convergence is likely, simply restart the job with **batch.sh &**. The model will use the results from the last successful iterations (stored in SCRTEMP) to restart.

Depending on the velocity law adopted, you may also need a file **RVSIG_COL**. This can be created using $cmfdist/exe/tlusty_vel.exe or $cmfdist/exe/wind_hyd.exe.

Some specialized cases are discussed below. These examples assume the **cpmod** command has been issued, and that you reside in the **r2** directory.

Case 1:

You wish to run a model, **r2** which only differs from **r1** in the number of depth points. You simply need to edit 2 lines in MODEL_SPEC (those containing ND and NP). In the VADAT file, **[LIN_INT]** should be set to .TRUE..

Case 2:

You wish to revise the number of super-levels in a model atom, or change the number of levels, from those used in model **r1**. Edit the MODEL_SPEC file to reflect the changes, and set **[LIN_INT]** to true in VADAT. You may also need to change the atomic data assignments in batch.sh, if using alternative data. If you are including many additional levels, several initial Λ-iterations might provide greater stability.

Case 3:

r2 is similar to **r1** except that you are changing one, or more, fundamental parameters (e.g., L). Edit the VADAT file to reflect the new value of L. Change **[LIN_INT]** to .FALSE., and make sure **[IT_ON_T]** is .TRUE.. This was the adopted procedure until very recently.

It is now possible to include a file (GREY_SCL_FAC_IN), taken from model r1, which contains T/T(grey) as a function of Rosseland optical depth. When present, this is used to scale T(grey) so as to provide a better estimate of the temperature structure. This is found to give a significantly better flux conservation. GREY_SCL_FAC_IN is obtained from GREY_SCL_FACOUT (see the GREY_TAU option description in VADAT description for more details).

Case 4:

You wish to include an ionization stage, or species, not included in model **r1**. This is one of the more difficult changes. Edit the batch.sh and MODEL_SPEC file to reflect the desired changes. You may also need to edit VADAT if the appropriate key-words have not previously been included.

To generate the required XzV_IN file do one of the following:

Method 1 (older method)

If it is a lower ionization stage, simply use the lowest existing ionization stage as the input departure coefficient file. For example, to include FeIII in a model, use FeIV_IN for FeIII_IN also.(It should also be possible to do the TX trick described below, but it is not yet implemented).

If it is a higher ionization stage, use DISPGEN in the **r1** directory to generate files containing excitation temperatures for each level and each species (WRTX option, with the generated files having a similar format to the departure coefficient files). Then use WR_F_TO_S (WRDC option) to create a new DC file. To include FeV in a model which has only FeIV, run WR_F_TO_S with the FeV oscillator file. For WRDC, use FeIVTX as the input excitation temperature file.

As an alternate, generate a departure coefficient file from another model, or perhaps from another species with a similar ionization potential.

For stability, the following works best (but may not always be necessary).

Include the species in the code with very low abundance (e.g., 10^{-12}). Perform enough Λ--iterations until the populations have stabilized. For an species with weak influence, it mat be best to set **[LIN_INT]** to .TRUE., so as not to effect the temperature structure.

Copy the XzVOUT files to XzV_IN files, and increase the abundance. Delete (or rename) POINT1, POINT2, SCRTEMP, and EDFACTOR. Perform enough lambda and full iterations until the populations have stabilized. At this stage, it may be better to set **[LIN_INT]** to .TRUE.. Repeat above procedure until the desired abundance has been reached. Initially the changes in abundance can be large, for example, a factor of 10^4. I generally go to the final abundance in a single step.

Method 2 (newer method)

To generate the EDDFACTOR and RVTJ files, run the existing model for 1 lambda iteration. Then edit MODEL_SPEC, VADAT, and batch.sh as for METHOD 1, and delete POINT* & SCRTEMP. In VADAT you will also need to set **USE_FIXED_J** to **TRUE**. Create the soft links for the atomic data files (i.e, batch.sh ass) and use $cmfdist/exe/guess_dc.exe to generate guesses for departure coefficients of the unknown populations. Now run the model for several lambda iterations. Then set **USE_FIXED_J** to **FALSE**, and run for several more LAMBDA iterations. If the species is not to important, you may then run a normal model iteration sequence. If the species will have a substantial influence on the temperature structure at depth, it may be better to rename the new *OUT files (for the new species only) to *_IN, delete SCRTEMP, and set LIN_INT to FALSE in VADAT. This will allow a new T structure to be determined when the model starts. NB: If the T structure does not need to be revised, simply start the model for 100 lambda iterations. If **DO_LAM_AUTO=T** (or is not set) in IN_ITS, CMFGEN will automatically switch, when appropriate, to computing a new J and non-lambda iterations.

Case 5:

You wish to use the hydrostatic structure from a TLUSTY run. To do this a file containing R, V and SIGMA (called RVSIG_COL for convenience) must be generated using **TLUSTY_VEL.EXE** (or some other program). The [VEL_LAW] is set to 7, [VEL_OPT] to RVSIG_COL, and [VINF] to the largest value in RVSIG_COL. The TLSUTY file *.11 (e.g., S40000g400v10.11) is required by **TLUSTY_VEL.EXE**. A program ($cmfdist/exe/rev_rvsig.exe) exist to allow changes to RVSIG_COL (e.g., changing number of grid points, new mass loss rate, new velocity law etc).

Computational Checklist for Starting a Model

1. Do I need to delete the POINT* and SCRTEMP file. These must be deleted for a new model, or for a model where you wish to use revise estimates of the populations, which will be obtained from the XzV_IN files?
2. Should I delete EDDFACTOR --- it must be deleted for a new model, or if changing the depth or frequency grid. It might also need to be deleted if restarting a model which has had problems.
3. Should I be using LIN_INT=T or LIN_INT=F?
4. How do I want to compute the initial estimate of the temperature structure?
5. Should **[XSLOW]** be T or F.
6. If using x-rays, have you set [MAX_CF] to >1000?
7. If you have changed Teff, is there additional species/ionization stages or processes that should be included.
8. Should I run several LAMBDA iterations first?

Computational Checklist for Running/Converged Model

1. Is the Rosseland optical depth at the inner boundary > 50 (ideally close to 100) to ensure LTE and the validity of the diffusion approximation at depth?
2. Has convergence been achieved (**OUTGEN, CORRECTION_SUM** and **STEQ_VALS** files).
3. Is flux conserved at all depths (OBSFLUX)? Convergence should typically be better than 2%.
4. Is the electron energy balance equation satisfied (**GENCOOL**), particularly in the outer layers of the model? This only needs to be checked when new physics is included, or in new parameter range.
5. Are there any non-standard error message or warnings in **OUTGEN**.

Trouble Shooting

CMFGEN is fairly stable, but parameter regimes are encountered where there may be convergence difficulties. Parameters controlling convergence, which are set in VADAT, have 'default' values chosen to ensure convergence rather than a high rate of convergence.

If CMFGEN halts unexpectedly the user should:

Check OUTGEN (and MODEL_SCR if it exists) for an error message. Hopefully most error messages are self-explanatory. Check **batch.log** for any Fortran errors that may have occurred.

Convergence difficulties can arise for several reasons.

1. You are moving from a low-ionization to a higher ionization model. In such cases an ionization front may develop in the wind. Across the ionization front, populations may change by orders of magnitude. In such cases, CMFGEN has trouble eating its way through the front. The solution of the transfer equation across the front is also not reliable. When the problem arises, it usually occurs with the ground state of a dominant species such as He II.

   Possible remedies:
   a. If possible, use higher ionization models as input.

   b. Restart the model with new input data (i.e. XzV_IN). Remove the fronts from the input files by hand. Use the **[LIN_INT]**=T option in VADAT to restart the model. Remember to delete (or rename) the POINT1* and SCRTEMP files.

      NB: The WRDC(OWIN=5,7,10,14) option in DISPGEN can be used to write out new DC files (called XzVDC by default) with depths 5 through 7, and 10 through 14 omitted. The absent depths will be recreated in CMFGEN through interpolation. Before using this option, make sure that the RVTJ and POPDUM files have been updated with the latest population estimates. This can be done by running CMFGEN for 0 iterations.

   c. Use **[INC_GRID]** and related options to insert extra points in the neighborhood of the ionization front. Note that this does not increase the number of points in the model, and hence the memory requirements. It is only for the solution of the transfer equation.

   Remember: it doesn't matter how you get the model to converge, only that you do.

2. Problems of convergence in the outer regions of the wind that appear to be temperature related.
   a. Fix the temperature (i.e., set **[FIX_T]=TRUE** in VADAT), and converge the model. Convergence with fixed T is generally rapid. Then set **[FIX_T]=FALSE** and try again.
   b. Insure that **[SCL_LN]=TRUE** in VADAT
   c. Increase the number of super levels. This seems to be particularly important at low wind densities (e.g., $M=10^{-7}$ $M_\odot$/yr).

3. Program computes a large negative luminosity, and perhaps crashes when computing the observed flux.

   Possible remedies:
   a. Ensure that **[FG_OPT]** is **INT/INS**.
   b. If the problem occurs on the last iteration, change the **[FRM_OPT]** to **INT**.
   c. Change **[METHOD]** option to **ZERO**, although **LOGMON** should be stable.
   d. Check validity of input data. Problem most often occurs when the populations associated with some strong resonance transition (e.g. C IV 1550) are way off. This can occur, for example, when you have used as input a CIV file in which the 2p state is not split, for a model in which it has been split. Use REWRITE_DC first (or a macro in an EDITOR) to update the XzV_IN input file.
   e. Use a finer spatial grid at the outer boundary.

   You can generally return (but not with the finer spatial grid) to the original option values once the model has begun to converge.

4. Poor model convergence and bad fluxes (as seen in OBSFLUX) at depth.

   Possible remedies:
   a. If a model with new stellar parameters, ensure that **[LIN_INT]** was FALSE when the model was started. If it was TRUE, restart the model (deleting EDDFACTOR, POINT*, and SCRTEMP).
   b. Check that the parameters, such as Mdot, used to create the RVSIG_COL file (if used) and in the VADAT file are compatible.

5. Convergence is proceeding smoothly (with correction possibly smaller than 5%), but then goes wild. Or changes start to systematically increase.

   Possible remedies:
   a. Do nothing, and continue iterating. The problem could simply arise because information from the optically thick regions of the wind needs time to propagate to the outer regions of the wind.
   b. Change the **[NEG_OPAC_OPT]** to **SRCE_CHK**. It's possible that the problem arose because some transition (generally some insignificant transition in the IR) has suddenly decided to laze.
   c. Force the linearization matrix to be recomputed --- This can be done by editing BAMATPNT, or by simply deleting BAMAT. The code will eventually do this anyway if it continues to detect that the changes are continuing to increase.
   d. Average the last 2 iterations, which can be useful is the corrections are oscillating in sign.

6. Poor convergence of a single (few) level at a single (few) depth.

   Possible Remedies:
   a. Rename the *OUT files to *_IN, making sure that the *OUT files are for the most recent iteration. Alter the bad departure coefficients to a more reasonable value, and recommence computation of the model. Remember to use the **[LIN_INT]=T** option in VADAT to restart the model, and move the POINT* and SCRTEMP files to a temporary subdirectory (in case something goes wrong, and you need them again).
   b. Include more depth points in the neighborhood of the instability.

c. Average successive population estimates, since the changes can alter in sign. This can be done using **$cmfdist/exe/do_ng_v2.exe**.

7. Asymptotic convergence is poor, with the maximum corrections remaining at the 1% level.

   Possible Remedies:
   a. Decrease number of "unimportant" levels if using cmfgen_dev.exe
   b. Pray for guidance.

Model Input Files

Model data

MODEL_SPEC: Parameter file for CMFGEN that specifies the following:

- The number of depth points and core rays.
- The species and ionization stages which are to be included in the model.
- The number of SUPER-LEVELS and FULL-LEVELS for each ionization stage. If using **cmfgen_dev.exe**, it also contains the number of IMPORTANT-LEVELS.
- The maximum number of overlapping lines: Generally set to 70 --- models with larger values may take longer to compute. It must be larger than the maximum number of lines whose Sobolev resonance zones (i.e. intrinsic line profiles) simultaneously overlap.

Every model must include **either** H or He.

Species should be included in order of increasing atomic number, while ionization stages should be included in numerical order.

For each species the final ionization stage (e.g. H II, He III, C V) should NOT be listed in MODEL_SPEC. The single level associated with the final ionization stage is automatically included by CMFGEN.

NB: Previously a change in ND, N_S or N_F, for any species, required CMFGEN to be recompiled and linked. Through the use of dynamic memory allocation this is no longer necessary. CMFGEN now only needs to be recompiled/linked when fixing bugs, adding new features etc.

VADAT: Main file specifying model parameters and options. The various options are explained later in this document.

IN_ITS: Specifies:

[NUM_ITS]: Number of iterations
[DO_LAMBA_IT]: If TRUE, does lambda-iteration.
[DO_LAMBDA_AUTO]: Automatically switch from Λ-iteratons?

This file may be edited while CMFGEN is running. Entering a 0 for NUM_ITS will halt CMFGEN after the next complete iteration. Entering a number larger than the value previously in the file will result in an additional

NUM_ITS(new) -NUM_ITS(old)

iterations. **[DO_LAMBDA_AUTO]** is optional, and is assumed to be TRUE.

HYDRO_DEFAULTS: Required if **[DO_HYDRO]** is set in VADAT. File is used to control iteration of the hydrostatic structure. This may be edited while program is running. Only **[N_ITS]** must be present. Some of the most important options are listed below. Others can be found in $cmfdist/new_main/do_cmf_hydro_v2.f.

[N_ITS]:	Number of iterations remaining.
[FREQ_ITS]:	Indicates how often hydrostatic structure is updated. Default is 8.
[STRT_ITS]:	Begin hydrostatic correction after iteration STRT_ITS. Default is 20.
[ATOM_DEN]:	Density at outer boundary for plane-parallel model. Gives indication how far to extend model.
[OB_OPT]:	Indicates how depth grid at outer boundary is specified (DEFAULT, SPECIFY). If SPECIFY, the grid locations are explicitly specified.
[NOB_PARS]:	Number of specified grid locations
[OB_P1]:	Grid location 1. If 20, last spacing if DTAU/20
[OB_P2]:	Grid location 2.

ROSSELAND_LTE_TAB: Required if **[DO_HYDRO]** is set in VADAT. Contains Rosseland mean opacity as a function of T & Ne. Can be computed using $cmfdist/exe/main_lte.exe. Ideally, it should be computed using the same model atoms and abundances as specified in VADAT and MODEL_SPEC.

XzV_IN: Estimates of departure coefficients as a function of depth. It is generally the XzVOUT file of a previously converged model, although they can be also created by an option(WRDC) in DISPGEN. Use **cpmod** to handle the create on of a new model. Alternatively, on Unix systems one can generate the XzV_IN files by doing the following:

```
    cp old/*OUT new/
    out2in  (simple procedure *OUT file to *_IN)
```

NB: The z, if present, is lower case (e.g., FeIII_IN).

The first non-blank line of XzV_IN contains a format date for the file. This is to allow for future format changes. The second line provides brief set of parameters relevant to the model and ionization species: the **stellar radius** (inner boundary), the **luminosity**, the number of **full levels** in the atom, and the number of **depth points** (ND). There then appears ND data sets, one for each depth, and ordered from the outer boundary to the inner boundary. Each data set is separated by a blank line. The first line of each data set contains the radius, the ion density, the electron density, the temperature, the ionization fraction, the velocity, the volume filling factor and the depth identifier (1 to ND). Only the first 4 quantities and the volume filling factor are utilized when starting a new model (but the other columns must be present). Subsequent lines contain the departure coefficients for each level in the FULL atom, ordered from 1 to NXzV_F.

T_IN: Estimate of the T structure of a model. Generally an XzVOUT file from a previous model. NB: The temperature will be scaled (if the appropriate option in VADAT is set) to allow for changes in the model parameters.

GAMMAS_IN: Estimate of mean ionization for each atomic species DUM. Generally the GAMMAS of a previously converged model. The file contains a series of data sets giving the electron density, radius, temperature, and the number of electrons per species in the model.

GREY_SCL_FAC_IN: Gives T/T(grey) as a function of Rosseland optical depth. Taken from previously converged model(GREY_SCL_FACOUT). When present it is used to scale T(grey) so as to provide a better estimate of the temperature structure for the first iteration. This is found to give a significantly better flux conservation.

RVSIG_COL: Needed when using **[VEL_LAW=7]** & **[VEL_OPT]=RVSIG_COL**. Contains R, V & SIGMA for model in column format. Use **$cmfdist/exe/tlusty_vel.exe** and **$cmfdist/exe/wind_hyd.exe** to create.

SCRTEMP: SCRTEMP provides the starting populations when it (and POINT1) are present. The file is only valid for the model for which it was created. If you want a model to use revised XzV_IN files, this file (and POINT1 and POINT2) MUST be deleted. Further discussed under 'Scratch Files'.

Atomic data files

HYD_L_DATA: Hydrogenic photoionization cross sections for `*l*' states.

GBF_N_DATA: Bound-free gaunt factors for hydrogen.

XzV_F_OSCDAT: Energy levels and oscillator strengths.

XzV_COL_DATA: Collisional data. Tabular format.

PHOTXzV_A: Photoionization data. Tabular format.

XzV_F_TO_S: Provides the links between the full-levels and super-levels. Only required when $N_S \neq N_F$. Use WR_F_TO_S to assist in creating these files.

DIEXzV: Dielectronic data: Presently taken from Nussbaumer and Storey.

TWO_PHOT_DATA: Data giving atomic data for 2-photon process. One file contains data for all species.

CHG_EXCH_DATA: Data giving charge exchange reaction rates. One file contains data for all species.

XRAY_PHOT_FITS X-ray photoioization cross-sections. One file for all species.

RS_XRAY_FLUXES Fluxes as a function of shock-temperature. Used when including x-rays in the model. Presently calculated using the old Raymond & Smith code. Only one data file ($cmfdist/misc/rs_xray_flux_sol.dat) is presently available, and was computed using solar abundances. Other data sets could be easily included.

Output Files

MODEL: Contains MODEL information, data from VADAT, and headers from the atomic data files. If code halts, check the MODEL_SCR and OUTGEN files for error messages. MODEL_SCR is converted to MODEL after a few seconds/minutes.

MOD_SUM: Brief formatted summary of the model. Useful for book-keeping and archival purposes.

OUTGEN: Summary of the results and corrections for each iteration. **Look at this file to check on the progress of a model, and for warnings and error messages.** Some warnings are generated all the time, and purely informational. The command

grep MAX OUTGEN

will return a list of the maximum corrections as a function of iteration. Similarly,

grep LUM OUTGEN

will return the radiative luminosity at the outer and inner boundaries as a function of iteration.

XzVOUT: Final departure coefficients for each model. Only output after final iteration. Can be created by running CMFGEN for 0 iterations. Can also be created from RVTJ and POPDUM files using DISPGEN. Same format as XzV_IN discussed earlier.

GAMMAS: Estimate of mean ionization for each atomic species DUM. Used for initiating new models.

RVTJ: Contains main atmospheric structure vectors, e.g., R, V, T, Ion and Atom population, Rosseland mean optical depth etc.. As with XzVOUT and the POPDUM files, it is only output after the final iteration. It can be created by running CMFGEN for 0 iterations. However in this case the mean opacities will be zero. This file is required by DISPGEN and CMF_FLUX. The format of the file is fairly obvious. For historical reasons, the populations of H & He are also output to this file, but never used.

POPDUM: Level populations for all (computed) ionization stages of species DUM (e.g., POPCARB, POPHYD). These files are required by DISPGEN and CMF_FLUX. The file format is fairly obvious with the following clarifications. The oscillator date is only used to provide a check that the correct atomic data is being used when running DISPGEN or CMF_FLUX. The populations of the ionization stages are listed sequentially in the file. Populations are listed for each level, then for each depth (d=1 is listed first). The final set of ND numbers associated with each ionization stage is the (SL) ion density, which is only used if the following ionization stage is unavailable. To read these files into another program, look at the read routines used by DISPGEN or PLT_SPEC.

OBSFLUX: Contains frequencies and observed fluxes. These are displayed by **PLT_SPEC**. OBSFLUX also contains information on how the luminosity varies with depth. This provides a check on the accuracy of the flux conservation. The spectrum in this file **SHOULD NOT** be considered as the final observed spectrum, although at present it must be used for the X-ray portion. Use CMF_FLUX to compute the observed spectrum.

The file contains a list of frequencies (in 10^{15} Hz) and then the list of the corresponding fluxes in Jansky's (assuming d=1kpc). The file then lists the radiative luminosity, dielectronic and implicit recombination line emission (if dielectronic lines are treated as individual lines), the total line emission (if note using blanketed option), the mechanical luminosity (if radiative equilibrium holds, L is not conserved in the CMF and this gives the correction to be made to the radiative luminosity), the Total Radiative Luminosity, and the X-ray luminosity. Ideally, the **total radiative luminosity** (radiative is the wrong word) should be constant. The radiative luminosity is given at each depth, while other terms are evaluated only for the shell centered at each depth. Finally we give a summary of the total X-ray luminosity emitted by the gas and the observed X-ray luminosity (which will be effected by absorption and by any intrinsic X-ray emission coming from the star/wind).

Diagnostic output files

CORRECTION_SUM: The number of correction greater than 100%, 10%, 1%, 0.1%, 0.01$ and 0.001% are output as a function of depth. This file is very useful. In most cases, the file will show that each depth has similar distribution of corrections, and that any differences changes fairly smoothly with depth. However in some models a few populations may behave unusually. For example, in the CORRECTION file, all corrections may be small except at one depth. This may indicate a convergence problem which can be corrected, either by hand, or using one of the correction procedures that are available.

EWDATA: Equivalent widths computed when using CMF of SOB modes. File is empty in BLANKETING mode.

CFDAT_OUT: Continuum frequencies --- not of much use.

GENCOOL: File containing HEATING and COOLING rates of the electrons for all the various processes (e.g., photoionization, recombination, collisional excitations and ionizations, X-ray cooling, adiabatic cooling). The net cooling rate should ideally be zero if the code is working correctly, and when the model is converged. In practice the use of super-levels prevents this from happening. Increasing the number of super levels and/or altering the level assignments should/can reduce the net cooling rate. Generally errors of 20% appear not to be important for most models. Ideally, the effect of these errors should be tested for models in the relevant parameter range. Typically the error is less than a few percent. At the inner boundary the errors may be larger but this does not matter providing the luminosity has been conserved (check OBSFLUX). The file format is somewhat similar to XzVPRR. **This file should be checked occasionally as it can reveal problems with the models or bugs in the code.**

HYDRO: Summary of the hydrostatic terms important for driving the wind. Output depends on the stellar mass as input through VADAT. At present, the MASS in VADAT only affects this file. HYDRO can be rewritten for a new stellar MASS using $cmfdist/exe/rev_hydro_turb.exe

J_COMP: Contains the value of the mean intensity at the inner and outer boundary as a function of frequency. Two mean intensities are output. One is computed using the ray by ray solution, the other using Eddington factors. Ideally they should be identical, in practice they differ by around 1% at the outer boundary. This file is only created on the final iteration. If a major crash occurs, it is often useful to rerun the code for 1 iteration so that this file is created. For very low mass-loss rate models, with large Rmax, J_COMP might reveal larger discrepancies in the outer boundary fluxes, particularly at infrared wavelengths. In such cases

you need to use a smaller step size at the outer boundary. Plt_jc_comp.exe can be used to plot J at the outer boundary.

JEW: Used when computing line equivalent widths. File is empty in blanketing mode.

LINEHEAT: Net cooling rates for each bound-bound transition. Defined as hv N_u A_{ul} Z_{ul} /4π, and it is thus the cooling per steradian. Because of the choice of program units, it is scaled by a factor of 10^{10}.

MEANOPAC: Summary of various optical depth scales (Rosseland, Flux, and electron scattering) as a function of depth. The optical depth scales have been explicitly corrected by the volume filling factor. The optical depth scales can be computed from the listed opacities using **dτ = -χf dz** where f is the volume filling factor.

NEG_OPAC: Lists each frequency, and the transition, for which a negative optical depth occurred. These negative optical depths arise due to population inversions, and generally (but not always) occur in the infrared. We have automatic procedures installed to handle these occurrences. They tend to occur more often when the model is unconverged.

NETRATE: Net rate, Z_{ul} (=1-J_{ul}/S_{ul}), for each bound-bound transition, ordered by increasing frequency. For each line, the net rate as a function of depth(1 to ND) is given.

PRRRXzV: Check file containing recombination and ionization rates for species XzV. If the code is working correctly, the total RATES for each species should be 0 (i.e. NET_RATE/TOTAL_RATE << 0.01 for a converged model). If this condition is not met, there is an ERROR.

STEQ_VALS: On each iteration, the value of each RATE (i.e., statistical equilibrium) equation at each depth is output. Tabulated as 'STEQ', with equation depth listed horizontally, and rate equation vertically. The format of this file has changed with the use of the development version. The first data set lists the statistical equilibrium equations for each ionization stage in sequential order. For a species with NXzV levels there at least NxZV+N where N is larger than 2. These extra equation relation to the ionization equilibrium, species conservation, and if present ionizations to excited states and Auger ionizations. The second data set list the merged rate equations in sequential order where degenerate equations have been removed. It has the same format as in the earlier vrsion of CMFGEN. Also output, under 'STEQ SOL', is the fractional correction to each population. This file can be very useful when diagnosing convergence difficulties. To facilitate interpretation of this file, a new diagnostic file CORRECTION_SUM is now created.

While the STEQ_VALS file is not user friendly it has improved. For example, to find a summary of corrections to T check the value of NT in the file MODEL. If this is 600, the command

grep "600(31)#" STEQ_VALS

will list the corrections to T for depths 31 to 40 as a function of iteration. In general MODEL can be used to find which equation corresponds to which species and super-level, and with a little more work, which atomic level. Similarly

grep "600(31)*" STEQ_VALS

will list the radiative equilibrium equation, which, ideally, should be zero. In practice, the final rate should be << than the initial value. Nb: The radiative equilibrium equation is et to zero when doing a LAMBDA iteration.

TRANS_INFO: Summary of all bound-bound transitions, in increasing wavelength order. The wavelengths are vacuum for λ < 2000Å, and in air for λ > 2000Å. Be careful --- some file list vacuum for λ > 2000Å.

TOTRATE: Total rate, $N_u A_{ul} Z_{ul}$, for each bound-bound transition. The statistical equilibrium equations, after the collisional terms are evaluated, are also output.

Scratch Files

These file are required while a program is running. They should be retained until a MODEL is fully converged.

POINT1: ASCII pointer file for scratch file, SCRTEMP. It points to the iteration that will be read in when a model is restarted. **In the event of convergence difficulties, it can be edited to point to an old iteration.** Say the model has gone crazy at iteration 25. You can return to iteration 23 (or some other iteration #) by simply changing the number above IREC and NITSF to 23. POINT1 also is used by the NG acceleration routines. The file is updated after each iteration.

POINT2: Backup copy of POINT1

SCRTEMP: Main scratch file. Saves all atomic populations after each iteration. It is used by the NG acceleration routines **and to restart an existing model.** FREE format, direct access file which may not NOT be portable without modification. Two formats are in use. The newer format allows a revised R grid to be stored for each iteration. For new models, this will be transparent to the user. However for some applications (using the DO_HYDRO option with an existing model) it may be necessary to rewrite the file into the appropriate format using REWRITE_SCR (or start as a new model).

EDDFACTOR: File containing the mean intensity J (RJ in program notation) for each frequency at each depth. Originally file contained the Eddington *f* values, hence the name. It and ES_J_CONV can be plotted using PLT_JH. Free format, direct access file which is (generally) NOT portable.

ES_J_CONV: Convolution of the mean intensity J with the Electron scattering redistribution function. Created when INCOHERENT electron scattering is assumed. Free format, direct access file which is (generally) NOT portable.

BAPNTMAT: Pointer and information file for BAMAT. If BAMAT and SCRATCH files are available, this file may be edited by hand so THAT CMFGEN does not recompute BAMAT etc. Useful when starting a stopped job. Normally, CMFGEN automatically sets the control switch.

BAIONPNT: Pointer and information file for BAION. This and BAION are no longer used.

BAMAT: Huge file which contains the LINEARIZED Statistical Equilibrium equations. Reading this file in when a model is nearly converged can decrease the model computation time considerably. Remember to delete the file after a model has completed. FREE format and NOT portable.

?_INFO:	Files indicating the size of direct access records in files such as EDDFACTOR, ES_J_CONV etc. They are needed by PLOT routines such as PLT_RJ, PLT_JH etc.
#SCRATCH###	Scratch file containing BAMAT inversion data. There is one file for each depth. They are used by CMFGEN_DEV.EXE to facilitate the solution of the large block of simultaneous equations which yield the corrections to the populations.

Explanation of fields in MODEL_SPEC

MODEL_SPEC is the top level control file for CMFGEN. With VADAT, it controls the nature and the type of model to be run. All parameters need to be included in this file.

[ND] This sets the number of depth points in the model atmosphere calculation. In most cases, the grid is computed internally. For W-R stars ND could be as low as 40. For O stars 60 points is recommended. When using VEL_OPT=7 (i.e., reading in a TLUSTY core hydrostatic structure) ND must be identical in MODEL_SPE & RVSIG_COL.

[NC] Number of rays strink core. Used for the angle integration. I typically use 10 to 15

[NP] Total number of rays. This is generally ND+NC. For some old options this must be ND+NC-2.

[NUM_BNDS] Number of bands used to in the linearization matrix. Choose 1 for a DIAGONAL operator and 3 for a TRIDIAGONAL operator.

[NCF_MAX] Maximum number of continuum frequencies. In BLANKETING mode, these frequencies also include lines. If NCF_MAX is too small CMFGEN will halt, and an error will be output to OUTGEN.

[MAX_SIM] The maximum number of lines whose profiles overlap. If MAX_SIM is too small CMFGEN will halt, and an error will be output to OUTGEN.

[NLINE_MAX] The maximum number of bound-bound transitions. In the original version, CMFGEN would halt if NLINE_MAX was too small. In CMFGEN_DEV, NLINE_MAX is computed internally, and [NLINE_MAX] in MODEL_SPEC is obsolete.

[NLF] Number of frequencies to be used across the Doppler core. Not used in BLANBKETING mode --- only by the CMF section.

[XzV_ISF] It indicates the level structure to be used for the atomic species XzV for CMFGEN_DEV. It requires 3 parameters and has the format

```
      10,20,30
```

where

- 10 is the number of important levels (≤NXzV).
- 20 is the number of super levels (= NXzV ≤ NXzV_F) in the model atom.
- 30 is the number of atomic levels (=NXzV_F) in the model atom.

For H, He, CNO, and perhaps Fe, it is a good idea to have the number of important levels identical to the number of super levels. To give the same convergence as CMFGEN set the number of important levels identical to the number of super levels for all species. For true impurity species, set number of important levels to 0.

[XzV_NSF] Obsolete reference used in MODEL_SPEC with cmfgen. It indicates the level structure to be used for the atomic species XzV for CMFGEN. It has two parameters and has the format

```
      20,30
```

where

20 is the number of super levels (= NXzV ≤ NXzV_F) in the model atom.

30 is the number of atomic levels (=NXzV_F) in the model atom.

If a weird error occurs when running CMFGEN, and it stops immediately, check that the usage of XzV_ISF and XzV_NSF is correct.

Explanation of options in VADAT

VADAT is the main driver file for CMFGEN. Some parameters need to be included even when they are not utilized. Some parameters need only be included when another specific parameter has been set to a specific value. For example, the parameters for the velocity law change depending on the choice of **[VEL_LAW]**.

All keywords in the following text are specified in bold between square brackets. Some parameters are checked for validity --- others are not. It is the responsibility of the user to ensure that the parameters are valid. Check the MODEL file after a job begins.

Keywords need not be in order, although it is recommended that the ordering of keywords not be changed dramatically from that provided. If a keyword can't be found, an error is output to OUTGEN, and program execution stops. Superfluous keywords (e.g., FIX_CIII when CIII is not included) are ignored.

Additional keywords are continually added to improve the accuracy, convergence properties, and applicability of the code. This will necessitate the VADAT file of old models be revised, if you wish to re-run the same model. This generally presents no difficulty, however, since the options are unique, and the code will inform you through the OUTGEN file when they are not present.

Options in VADAT are read in via the routine
new_main/mod_subs/rd_control_variables.f.
This routine can checked for option ordering, and additional info.

Options for Atmospheric Structure

[RSTAR] Radius of star (i.e. inner boundary of model) in program units of 10^{10} cm. In these units the radius of the Sun is 6.96. The optical depth at **[RSTAR]** is velocity and mass-loss rate dependent, and can be found using DISPGEN. The user should check that the code extends sufficiently deep (i.e., τ_{Ross}=10 to 100) so that LTE is recovered. Going unnecessarily to (τ_{Ross}=1000) may cause convergence difficulties. τ_{Ross}(max) is now output to CMFGEN in the first iteration when the **[LIN_INT]** option is false.

[RMAX] Outer radius of star in units of **[RSTAR]**. For low density atmospheres **[RMAX]**=100 is adequate, while for W-R stars **[RMAX]**=200 is suggested. The strength of some lines (e.g., He I 5876, 10830) may be weakly affected by the choice of **[RMAX]**. The strength of forbidden lines formed at low densities may be substantially affected.

[DO_HYDRO] Indicates that the density structure in the photosphere is to be iterated on so as to better to satisfy the hydrostatic equation. If T, HYDRO_DEFULTS muse be present as a separate file, and **[VEL_LAW]** must be 7. In this case both **[VINF]** and **[BETA]** must also be given in VADAT.

[VEL_LAW] Indicates which velocity law to adopt. New velocity laws can be added to the code by utilizing this option. Each velocity law option has its own set of compulsory keywords.

[VEL_LAW]=3 Standard β-velocity modified at depth so that it approaches a hydrostatic structure. The velocity law has the form:

$$v(r) = \left(V_o + (V_\infty - V_o)(1 - R_*/r)^{\beta} \right) \; / \; \left(1 + V_o/V_{core} \exp([R_* - r]/h_{eff}) \right)$$

[VCORE] Velocity in km s^{-1} at R_* when $V_o >> V_{core}$. Typically less than 1 km s^{-1}.

[VPHOT] Generally referred to as the photospheric velocity, but its exact meaning depends on the values adopted for the other parameters (V_o , in km s^{-1}).

[VINF] Terminal velocity of the flow in km s^{-1}.

[SCL_HT] Scale height (h_{eff}) of photosphere in units of RSTAR. Specifies density structure at low velocities. Can be used to specify a velocity structure which is approximately hydrostatic.

[BETA] Speed of velocity law. That is β in the usual β-velocity law. Typical values are in the range 0.5 to 4.

[VEL_LAW]=4 Reads in R,V & SIGMA from a file (simple column format). No options.

[VEL_LAW]=6 β-velocity modified at depth so that it approaches a hydrostatic structure. In the outer regions it is modified so that it can have an extended acceleration zone. The TSTV option in DISPGEN can be used to examine the shape of the velocity law for different parameter combinations. The velocity law has the form:

$$v(r) = \left(V_o + (V_\infty - V_{ext} - V_o)(1 - R_*/r)^{\beta 1} + V_{ext}(1 - R_*/r)^{\beta 2} \right) \; / \; \left(1 + V_o/V_{core} \exp([R_* - r]/h_{eff}) \right)$$

[VCORE] Velocity in km s^{-1} at R_*. Typically less than 1 km s^{-1}.

[VPHOT] Photospheric velocity (V_o) in km s^{-1}.

[VINF1] Terminal velocity of flow in km s^{-1}, of the first component of the velocity law.

[SCL_HT] Scale height (h_{eff}) of photosphere in units of RSTAR. Specifies density structure at low velocities. Can be used to specify a velocity which is approximately hydrostatic.

[BETA1] Speed of velocity law. That is β in the usual β-velocity law. Typical values are in the range 0.5 to 4.

[EPPS1] Needed when $\beta_1 < 1$. Chosen so that $(1-\varepsilon_1 R_*/r)$ is greater than zero at the core, and hence so that dv/dr is finite.

[VINF2] Terminal velocity of flow in km s^{-1}. If **[VINF2]=[VINF1]**, the second component of the velocity law has no effect.

[BETA2] Speed of the second component of the velocity law. That is β in the usual β-velocity law. Typical values are in the range 5 to 50.

[EPPS2] Needed when $\beta_2 < 1$. Chosen so that $(1-\varepsilon_2 R_*/r)$ is greater than zero at the core, and hence so that dv/dr is finite.

[VEL_LAW]=7 R, V and sigma (= dlnV/dlnr-1) are read in from a file. R_{max}/R_* should agree with the value specified in the VADAT file. R_* is scaled to agree. Presently no interpolation is done, and the R values read in define the adopted radius grid. Create using **$cmfdist/exe/tlusty_vel.exe** or **$cmfdist/exe/wind_hyd.exe**.

[VEL_OPTION]
Indicates from which file velocity data is to be read. Two options available: RVSIG_COL (simple column format) and deKOTER (file in Alex deKoters format). See newsubs/rd_rv_file_v2.f for further details.

[VINF] Terminal velocity in km s^{-1} of wind. Should be similar to value in file.

[VAR_MDOT] Is the mass loss rate going to vary with time, and hence radius. For modelling LBVs, such as AG Car.

[VM_FILE] File with density and clumping info for model with variable MDOT.

[VEL_LAW]=10 Velocity law for SN models. A power law in r is (generally a Hubble law) is assumed.

[VCORE] Velocity at inner core (km/s).

[BETA1] Exponent for velocity law. Use 1 for a Hubble Law.

[RCUB_RHO] Density*(core radius)^3. The density is in gm/cm^3, while the core radius is assumed to be in program units (i.e., 10^10 cm).

[N_RHO] Exponent for power law variation of density. For SN, N_RHO should be of order 10.

[VEL_LAW]=11 For SN models using a hydrodynamic structure.

[VINF] Terminal velocity, in km s^{-1}, of moel. Should be similar to value in file.

[MDOT] Mass-loss rate in units of M_{sun}/yr.

[LSTAR] Total luminosity of star in units of L_{sun}. If the hydrostatic structure is updated, it we be automatically be edited in VADAT by CMFGEN to be consistent with **Teff** and **R(Teff).**

[TEFF] Effective temperature (in units of 10^4 K) of star. Only used when hydrostatic structure is updated. For a spherical star, TEFF is specified at Tau=2/3. For plane-parallel model, RSTAR is used to defined TEFF.

[LOGG] Log of surface gravity (cgs units). Only used when hydrostatic structure is updated. For a spherical star, **log g** is specified at Tau=2/3. For plane-parallel model, RSTAR is used to defined **log g.**

[MASS] Mass of star in units of M_{sun}. Presently this parameter is only used for output to HYDRO. If the hydrostatic structure is updated, it we be automatically be edited in VADAT by CMFGEN to be consistent with **log g** and **R(Teff).**

[DO_CL] Switch to turn clumping on/off. A simple filling factor approach is used. Clumping currently ONLY works in BLANKETING mode. Incorrect results will be obtained if clumping is used in CMF or SOB mode, or if dielectronic lines are included as pure lines. In order to generate a FLUX spectrum, the code does not halt when **[FLUX_CAL_ONLY]** is specified with **[SOB]** for some (or ALL) lines.

[CL_LAW] Character string which specifies how to evaluate the clumping factors. Currently only a single law, EXPO, is available. No effect if **[DO_CL]**=FALSE.

[N_CL_PAR] Number of clumping parameters. For the **[CL_LAW]**=EXPO, this value should be 2. No effect if **[DO_CL**]=FALSE.

[CL_PAR_1] Clumping parameter (i.e., filling factor) at V_∞. Typically choose 0.1. To preserve the same spectrum as an unclumped model, the mass loss rate should be multiplied (and hence reduced) by a factor SQRT(**[CL_PAR_1]**). No effect if **[DO_CL]=**FALSE.

[CL_PAR_2] Indicates how rapidly clumping should be switched on. It is assumed to be damped at low velocities. Parameter is specified in km s^{-1}. Typically we adopt a few hundred km s^{-1} for a W-R star. No effect if **[DO_CL]=**FALSE.

[DUM/X] When **+ve**, it gives the abundance of species DUM, by number, relative to some arbitrary species X. This mode tends to be most useful for species modified by nuclear processes (e.g., H, He, C). When **-ve**, it specifies the mass fraction of the species. This mode is useful for species whose mass fraction is not affected by evolution (e.g., Fe). The 2 modes may be mixed. DUM should be replaced by HE, CARB, NIT etc. i.e., the DUM variables specified in the MODEL_SPEC file, and in CMFGEN.

SN model options

[REV_RGRID]	Indicates whether R grid should be automatically revised, after each iteration. Allows better treatment of H ionization fronts.
[RG_TYPE]	Type of new R grid (UNIFORM of FIX_NX)
[N_RG_PAR]	Number of parameters used to help specify the new grid.
[RG_PAR_1]	Parameter 1
[RG_PAR_2]	Parameter 2 etc.
[JG_W_V]	Include velocity terms when evaluating initial grey temperature structure.
[DO_DDT]	Include comoving derivative terms in the statistical equilibrium equations.
[TS_NO]	Sequence number for super novae model, beginning with model 1. Model 1 must be computed ignoring time derivatives.
[SN_AGE]	Age of SN in days.
[INC_RAD_DEACYS]	Include radioactive decays. For use with time-dependent radiative transfer models.
[REL_OBS]	Include all relativistic terms in the observer's frame solution.
[REL_CMF]	Include all relativistic terms in the CMF solution for the observed intensity.

Options for continuum frequency grid

[RD_CF_FILE] Read in continuum frequencies from file, perhaps generated by an earlier model. Option rarely utilized since blanketing installed.

[MIN_CF] Minimum continuum frequency (if calculating) in program units of 10^{15} Hz. Bound-bound transitions at lower frequencies are neglected in the blanketing calculations. Example, for W-R star use: 3.49897 10^{-3}

[MAX_CF] Maximum continuum frequency (if calculating) in program units of 10^{15} Hz. This value should be 1.5 or more times the highest ionization edge of all included species. For W-R stars typically adopt a value of 50. A much higher value needs to be adopted when X-rays are included.

[FRAC_SP] Fractional spacing for small frequencies. Typically adopt 1.1. Thus $\nu_{i+1} = \nu_i$ / **[FRAC_SP]**.

[AMP_FAC] Amplification factor for large frequency ranges --- typically adopt 1.05. Thus $\Delta\nu_{i+1} = \Delta\nu_i$ x **[AMP_FAC]**.

[MAX_BF] Maximum frequency spacing in program units of 10^{15} Hz close to bound-free edges for frequencies > 10^{15} Hz. Typically we adopt 0.10D0. Too large a value will influence the accuracy with which recombination rates are computed.

[FR_GRID] (Hidden). When non-zero, it allows earlier techniques to be used to compute the frequency grid. When specified, 0 uses the latest grid option.

[DO_DIS] Allows for level dissolution. This leads to better behavior near bound-free edges, and is more realistic. Usually set to TRUE.

[dV_LEV] Spacing in km s^{-1} on low side of bound-free edge. This option is to insure good frequency spacing when level dissolution is in effect. Typically adopt 200.0 km s^{-1}.

[AMP_DIS] Amplification factor on low side of bound-free edge. As we move away from the bound-free edge (to lower frequencies) the frequency spacing increases by **[AMP_DIS]** until next continuum frequency is reached (Use 1.4?)

[MIN_DIS] Minimum frequency in program units of 10^{15} Hz for level dissolution. Below this frequency we make no special allowance for level dissolution in choosing the continuum frequencies. Use 0.1.

[CROSS] If TRUE, continuum cross-sections are evaluated at all frequencies. If FALSE, continuum cross-sections are evaluated at the pure continuum frequencies, and additional frequencies as determined by **[V_CROSS]**. The FALSE option can improve the speed of the code by a factor of 3 (or more). Tests indicate that setting **[CROSS]**=FALSE does not generally affect the accuracy of the model calculation. FALSE is the preferred setting.

[V_CROSS] Maximum separation, in km s^{-1}, between evaluations of the continuum opacity and emissivity. Typically adopt 750.0 km s^{-1}. This value should be compatible with the smoothing adopted for the photoionization cross-sections and **[SIG_GAU_KMS]**. It is also used in defining the frequency grid.

[SIG_GAU_KMS] Sigma of Gaussian (in km s^{-1}) used to smooth the photoionization cross-sections. As most of the current files have already been smoothed with a resolution of 3000 km s^{-1}, this option will generally not have any effect if **[SIG_GAU_KMS]** is set below 3000 km s^{-1}. Some unsmoothed, or lower smoothed, photoionization files are available. Eventually all the photoionization data will be unsmoothed so as to provide greater flexibility.

[FRAC_SIC_GAU] Hidden parameter which indicates the spacing (in sigma) used for the numerical smoothing. Default is 0.25.

[CUT_ACCURACY] Hidden parameter: After smoothing, unnecessary grid points in the photoionization cross-sections are deleted. Points are only deleted when the cross-section can be interpolated, using linear interpolation, from neighboring points with a fractional accuracy of [CUT_ACCURACY]. The default value is 0.02. This value is generally smaller than the accuracy of the photoionization cross-sections.

[ABV_EDGE] (Hidden). Uses only data above photoionization edge when smoothing. Default is TRUE.

[EXT_LINE_VAR] Extent of variation region beyond resonance zone measured in terms of V_∞. I typically adopt 0.5.

[ZNET_VAR_LIM] Iterate on net rates at those depths where ABS(ZNET-1) < ZNET_VAR_LIM. Typically set to 0.01. When ABS(ZNET-1) is small, the line is essentially optically thin.

[WNET] If TRUE, we iterate on the net rates (rather than use full linearization) for weak lines.

[WK_LIM] Used as a control parameter for WNET. When set to 0.1, lines with maximum line opacity to continuum opacity of < 0.1 are treated using net rates.

Computation of radiation field

[PP_NOV] Hidden: Use plane-parallel geometry WITHOUT velocity field? Default is FALSE (i.e., spherical model).

[PP_MOD] Hidden: Use plane-parallel geometry with velocity field? Default is FALSE (i.e, use spherical model).

[INCL_DJDT] Hidden: Include DJDt terms in transfer equation for SN models. For Hubble flow only. Defaults if FALSE.

[USE_DJDT_RTE] Hidden: Allows the user to force the DJDt transfer routines to be used, even when the DJDt terms are not to be included. Useful to testing, and should also be used for the first model of a time sequence.

[DJDT_RELAX] Hidden: Relaxation parameter to scale DJDT terms to assist initial convergence. Default is 1 (i.e., no relaxation.). Parameter was used for initial model development.

[USE_J_REL] Hidden: Use MOM_J_REL_VN to solver CMF transfer equations. Relativistic terms may be included. Defaults if FALSE.

[INC_REL] Hidden: Include relativistic terms in the transfer equation. USE_J_REL must be TRUE. Default is FALSE.

[INC_ADV_TRANS] Include the advection terms in the transfer equation. Default is generally FALSE, but it is TRUE when both USE_J_REL and INC_REL are TRUE.

[USE_FIXED_J] Tells CMFGEN to use a previously computed J as stored in EDDFACTOR. When TRUE, the calculated observed spectrum is meaningless. Set to TRUE when installing new-species. This allows populations to be rapidly computed that are consistent with the radiation field. Can only be TRUE when doing a LAMBDA iteration. Also used in CMF_FLUX to save computational effort (where you use an old J to provide an estimate for the electron scattering source function).

[JC_W_EDD] Use Eddington factors to compute JBAR for lines. For use with the CMF option. Set to TRUE. Not utilized in pure SOB or pure BLANKETING modes. Alternative modes, which may still work, are obsolete and are slower.

[NOV_CONT] In non-blanketed mode, ignore velocity terms when computing continuum.

[JBAR_W_EDD] Compute line continuum intensity using Eddington factors

[DIF] Indicates whether the diffusion approximation is to be used at the inner boundary. Alternative is a Schuster-like boundary condition that hasn't been utilized for ages, and may no longer work.

[COH_ES] Switch for coherent electron scattering. For best convergence set key to TRUE. For flux calculations, particularly in LBV models, set to FALSE. Work on improving the convergence in NON-COHERENT mode is ongoing.

[OLD_J] Obsolete: Use old J to provide estimate for J_ES.

[MIX_COH] Mix coherencies in variation of J. Tells CMFGEN to assume that the electron scattering is coherent at some depths, as determined by **[ES_FAC]**, when computing the variation of J. Under development.

[ES_FAC] Determines how close RJ (mean intensity) and RJ_ES (scattered mean intensity) have to be to use the coherent approximation when computing the variation of J. Use **[ES_FAC]**=0.1. Under development.

[N_TYPE] In the computation of J using the moment equations the moment N (in the moment set J, H, K, N) must be specified. This could be done using the Eddington factor N/H but this is unstable as H may go through zero.

N_ON_J
: Use the Eddington factor N/J at all depths. Preferred option in CMFGEN.

MIXED
: Use the Eddington factor N/H except at those depths where it is undefined (e.g., where H is close to zero). At those depths, N/J is used.

G_ONLY
: Use the Eddington factor ***g*** = N/H at all depths. In blanketed models this option is can CRASH the code. I tend to use this option in CMF_FLUX.

[FG_OPT] Determines the method used to solve the radiative transfer equation (RTE) in the *(p,z)* coordinate system. The solution of the RTE is used to compute the Eddington factors ***f*** and ***g*** needed to solve the moment equations.

INT/INS
: Preferred setting. Uses the integral short characteristic approach(INT) to solve the RTE. `/INS' indicates that extra points are inserted near z=0. It may be omitted. `INT/INS' has greater stability than `DIFF/INS' since the intensity, I, is always guaranteed to be greater than zero.

DIFF/INS
: Uses the difference approach to solve the RTE. Original approach. Generally fairly stable but can get problems on route to a converged model.

Accuracy options

[METHOD] Method used to estimate optical depths. A Value of ZERO indicates that the optical depths are to be estimated using a pure Trapazoidal rule. Can be useful if model is suffering convergence difficulties because of an ionization front.

LOGMON
: Preferred option. Optical depths estimated by the trapazoidal rule with a correction based on the first derivatives using the Euler-McLaurin summation rule. The derivatives are estimated using a cubic that is forced to be monotonic over each integration interval.

LOGLOG
: Optical depths estimated by the trapazoidal rule with a correction based on the first derivatives using the Eurler-McLaurin summation rule. The derivatives are estimated using the stable approximation

$$(d\chi/dr)_i = (\chi_i/r_i)(\ln \chi_{i-1} - \ln \chi_{i+1}) / (\ln r_{i-1} - \ln r_{i+1})$$

LOGLIN
: As for LOGLOG except derivatives estimated using

$$(d\chi/dr)_i = \chi_i(\ln \chi_{i-1} - \ln \chi_{i+1}) / (r_{i-1} - r_{i+1})$$

LINLIN
: As for LOGLOG except derivatives estimated using

$$(d\chi/dr)_i = (\chi_{i-1} - \chi_{i+1}) / (r_{i-1} - r_{i+1})$$

[VFRAC_FG] Used to facilitate the inclusion of extra points in FG_J_CMF_V9 --- the default procedure used to compute the Eddington factors. FG_J_CMF_V9 solves for J & K using the ray

method. This option was installed to overcome numerical difficulties, and is primarily for CMF_FLUX. If set to **m** (for example), extra points are inserted along each ray to ensure that the velocity step size is less than a **m** local Doppler width. In CMFGEN I usually omit by setting to a large value (e.g., 2000). This option, can be used with the current version of cmfgen-dev.exe

[VFRAC_MOM] Used to facilitate the inclusion of extra points in MOM_J_CMF_V6. MOM_J_CMF_V6 solves for J & K using Eddington factors. This option was installed to overcome numerical difficulties, and is primarily for CMF_FLUX. If set to **m** (for example), extra points are inserted along the radius grid to ensure that the velocity step size is less than a **m** local Doppler width. In CMFGEN I usually omit by setting to a large value (e.g., 2000). It is unclear whether convergence would be obtained with the current version of cmfgen-dev.exe. The linearization section presently does not include extra points.

[THK_CONT] Switch to utilize the thick boundary condition for the computation of the continuum. In blanketing mode the atmosphere is extended by extrapolation. In other modes a crude approximation is utilized. Preferred default is TRUE --- this gives a smooth and more realistic run of properties at the outer boundary.

[TRAP_J] Method to use for the computation of weights for the calculation of the moments J, H, K, and N. **[TRAP_J]**=T is the preferred option. This indicates to assume a linear approximation for the specific intensity I between each node. For J this is equivalent to a trapazoidal rule. For other moments the appropriate weight (μ, μ^2, μ^3) is specifically taken into account when computing the weight.

[OBC_TYPE] Hidden: Outer boundary condition type. Default is 1.

[BC_PAR1] Hidden: Frequency (10^15 Hz) below which new boundary condition is adopted.

[INCID_RAD] Hidden. Include incident radiation on outer boundary (for use with plane-parallel models).

Line options

[TDOP] Presently the line absorption profile is assumed to be a DOPPLER profile that is independent of depth and the atomic species. The width of the Doppler profile depends on 3 parameters --- the adopted electron temperature **[TDOP]** in program units of 10^4 K, the adopted atomic mass in a.m.u. [AMASS_DOP], and the turbulent velocity **[VTURB]**. One day, when bored, I will update CMFGEN, to use variable Doppler widths etc.

[AMASS_DOP] Atomic mass (in a.m.u) used to compute the Doppler profile. At present this is the same for all species at all depths. The best approach is probably to set **AMASS_DOP=1.0D+40**. Then use VTURB to control the width of the line absorption profile.

[VTURB] Turbulent velocity, in km s^{-1}, used to compute the line absorption profile. At present this is assumed to be depth independent, and the same for all species.

[MAX_DOP] Maximum half-width of resonance zone in Doppler widths. Because of the possibility of very strong lines, a value of 6 is used. For weak lines a smaller value could be utilized, but at present all lines use the same value.

[FRAC_DOP] Spacing in CMF resonance zone in Doppler widths. For statistical equilibrium calculations, particularly model grid calculations, **use 1.0**. Because of numerical instabilities, a smaller value may not give increased accuracy. The presence of instabilities depends on the both the spatial and frequency grid scales, and the adopted Doppler (thermal + turbulent) velocities. We are trying to develop automatic methods to better handle the instabilities. For the observed flux calculations use 0.5, together with VFRAC_FG and VFRAC_MOM set to 1. This gives more accurate profiles with less bleeding to the red. Note that VFRAC_FG and VFRAC_MOM only directly effects the calculation in the comoving-frame. In the observer's frame it affects the computed spectrum via the electron-scattering emissivity.

[dV_CMF_PROF] Frequency spacing in km s^{-1} across the CMF profile (i.e., from the red edge of the resonance zone to $+2V_\infty$). Utilized primarily in the statistical equilibrium calculations. Use a value a few times that of the DOPPLER width. When the final flux calculation is performed this is reduced to FRAC_DOP*DOPPLER_WIDTH (if **[INS_F_FORM_SOL]** is TRUE).

[dV_CMF_WING] Frequency spacing in km s^{-1} in the electron scattering line wings of CMF profile. Generally use a few hundred km s^{-1}.

[ES_WING_EXT] Extent of non-coherent electron scattering wings beyond the resonance zone in km s^{-1}. 2500 km s^{-1} is satisfactory.

[R_CMF_WING_EXT] Extent of coherent electron scattering wings beyond resonance zone (in units of V_∞). When electron scattering strongly

influences the profiles, a value of 3.0 should be used. The option allows for the fact that in an expanding atmosphere electron scattering always increases the wavelength of a photon (assuming COHERENT scattering only).

Options for calculation of spectrum in observer's frame.

[OBS_EXT_RAT] Half-width of observed profile in units of V_∞. Value must be ≥ 1.0. Typically adopt 1.1

[dV_OBS_PROF] Frequency spacing in km s^{-1} across observed profile. Typically one Doppler width.

[dV_OBS_WING] Frequency spacing in km s^{-1} in electron scattering line wings. 200 km s^{-1} is reasonable.

[dV_OBS_BIG] Frequency spacing in km s^{-1} between lines i.e., in the continuum. Your choice. Typically we adopt 2000 km s^{-1}.

[FLUX_CAL_ONLY] Switch to indicate to CMFGEN that it should undertake a pure FLUX calculation i.e., it should compute the observed spectrum. No corrections are made to the atomic populations in this mode. To compute a CONTINUUM spectrum, set this option to TRUE and **[GLOBAL_LINE]** to SOB. To compute the He2 (i.e. He II) spectrum set this option to TRUE, **[GLOBAL_LINE]** to NONE, **[TRANS_He2]** to BLANK, and **[TRANS_XzV]** to SOB (all other species). **This option, and the following 4 options, are now obsolete in CMFGEN. These tasks are now performed in CMF_FLUX. This option must be FALSE when computing a full model. Options have the same meaning in CMF_FLUX_PARAM file for CMF_FLUX.**

[EXT_FRM_SOL] Extend formal solution, by extrapolation of the opacity and emissivity, a factor of 10 in R. Useful to see whether the choice of RMAX is influencing the OBSERVED spectrum.

[INS_F_FRM_SOL] Insert extra frequencies into the formal solution. These extra frequencies are inserted to improve the line profile computation. Set to TRUE.

[FRM_OPT] Method for evaluating OBSERVERS frame spectrum using a pure comoving-frame approach. Options are **INT** and **DIFF**, which have the same meaning as for **[FG_OPT]**. INT is slower, but more stable.

[DO_SOB_LINES] Calculate line equivalent widths when doing Sobolev calculation.

[SOB_FREQ_IN_OBS] Consider lines treated in Sobolev mode when computing the continuum frequency set.

[LAM_SET] Switch to SOBOLEV option for lines with wavelengths smaller than F_LAM_BEG or greater than F_LAM_END. We use the GLOBAL option for lines with F_LAM_BEG < λ < F_LAM_END. For this option, F_LAM_BEG is normally zero. Don't use with CLUMPING. Useful for computing the observed flux of a small spectral region with CMF_FLUX.

[F_LAM_BEG] If [FLX_CAL_ONLY] is TRUE, it is the wavelength (in Angstroms) at which we begin the flux calculation with lines. It is also used with the LAM_SET option. Note that the continuum flux is computed at wavelengths shorter than F_LAM_BEG.

[F_LAM_END] If [FLX_CAL_ONLY] is TRUE, it is the wavelength (in Angstroms) at which we end the flux calculation. It is also used with the LAM_SET.

[VERBOSE] Hidden: Indicates that additional error meassage, warning etc to be output. Options is not fully implemented. Default if False.

Options controlling the treatment of bound-bound transitions.

[GLOBAL_LINE] Switch to indicate which modes are to be used to compute the net-rates (etc) for individual line transitions.

BLANK All lines treated in blanketing mode

SOB All lines treated using the SOBOLEV approximation. Use this model for calculation of the continuum spectrum, or a Sobolev model.

CMF All lines treated in the CMF but in NON-BLANKETED mode. This option is becoming obsolete. Use SOB option for fast-dirty models, and the BLANK option for sophisticated modeling.

NONE The computation mode for lines from EACH species XzV is specified by **[TRANS_XzV]**. Use this mode to examine the effect of lines due to a particular species (on a model or on the observed spectrum). The direct influence of individual lines on the observed spectrum is now done better with CMF_FLUX.

[GF_CUT] Omit lines with ***gf*** < **[GFCUT]** and lower level greater than GF_LEV_CUT. At present used only for species with an atomic No > [AT_CUT]. Useful for neon, and higher elements.

[GF_LEV_CUT] Only omit transitions to levels, in each ion, if their lower level sequence number > **[GF_LEV_CUT]**. Normally set to a low number like 10, although 0 is valid. This option has been partially superceded by **[MIN_TRANS]**.

[AT_CUT] Allows lines meeting the **[GF_CUT]** criterion to be omitted provided the elemental atomic number is ≥ **[AT_CUT]**.

[MIN_TRANS] This gives the minimum number of downward transitions from a level that MUST be included before any transitions are omitted from the calculation. A non-zero value for this option ensures that no important transitions are omitted, even if they are very weak. Typically set to 10, but could be lower.

[THK_LINE] Use thick line boundary condition in CMF mode. Preferred option is TRUE.

[CHK_L_POS] Check for negative line opacity in CMF and SOBOLEV modes. Necessary as the radiative transfer equation, as formulated, is unstable to switches in the sign of the opacity. If TRUE, the line opacity is adjusted to ensure that the total opacity remains positive. Usually affects only weak lines in the IR. Preferred option is TRUE, except (perhaps) in SOBOLEV mode.

[**NEG_OPAC_OPT]** Option for treating negative opacities in BLANK mode. Two options presently available: **SCRE_CHK** and **ESEC_CHK**. **ESEC_CHK** was the previous default. Basically it sets the total opacity to 0.1*ESEC (electron scattering opacity) when, as a consequence of a negative line opacity, it falls below this value. **SRCE_CHK** was introduced for some O star models because the line opacity for some far IR lines (e.g. H(9-8)) could become negative (or very small) during the iteration process, while their (absolute) Sobolev optical depth was still large (i.e. 10^5). In such cases the **ESEC_CHK** option caused problems because the SOURCE function became much too large. **ESEC_CHK** is preferred, except when there is a problem (see trouble shooting section).

[He2_RES=0] Set rates in He II resonance lines to zero? Obsolete option not utilized. Set to FALSE.

[ALLOW_OL] Include line overlap in SOBOLEV approximation. Line overlap is included only crudely.

[OL_DIF] Maximum velocity difference (km s^{-1}) for overlapping lines. Typically adopt 50 km s^{-1}. Only of use with the SOBOLEV approximation.

[SCL_LN] Scale the line cooling/heating rates before adding to the radiative equilibrium equation. Set to TRUE. This option adjusts for the fact that the energy levels in a super-level do not have exactly the same energy. Forcing the levels in a SL to have the same departure coefficient can introduce an artificial heating/cooling term. The cooling/heating rates are scaled by the ratio of the mean wavelength to the actual wavelength. Especially important in O star winds where scattering dominates over collisional processes. It can also be important in cases where only a few super-levels per ion are used.

[SCL_LN_FAC] Performs the **[SCL_LN]** scaling only if the lines lie within a factional spacing of **[SCL_LN_FAC]**. Set to 0.5.

[SCL_DEN_LIM] Hidden: switches off the scaling of the line cooling rates when the electron density exceeds SCL_DEN_LIM. Default value is 10^30 (i.e., don’t switch off).

Physical process to be included

[INC_CHG] Include charge exchange reactions --- with hydrogen and helium. Can be important in models where the neutral hydrogen or helium fraction is greater than 10^{-4}. Can be set to TRUE for all models, but in most O and WR models it is generally set to FALSE.

[INC_TWO] Include two photon processes (e.g., decay from the 2s ^{2}S state of H). Set to TRUE.

[INC_RAY] Include Rayleigh scattering for H. Accurate longward of Lya, but changes needed at shorter wavelengths. In practice, this should make little difference as very little flux emitted at these wavelengths when Rayleigh scattering is important. Rayleigh scattering due to neutral He and He+ has not yet been included.

[INC_AD] Include adiabatic cooling. Routine was recently revised to improve convergence and accuracy. This option should only be included when **[INC_ADV]** is T.

For many models this option can be set to FALSE. For low-mass loss rate models, adiabatic cooling can be important for the temperature structure although its effect on the spectrum may be small. Check GENCOOL file to see if adiabatic cooling should be included — the relevant terms are output even if switched off. If IN_ADV is true, and if adiabatic cooling is important, convergence will be slower. This is expected since the temperature structure is strongly coupled to deeper depths even in the optically thin region of the stellar wind. In addition populations of impurity species that are coupled to the temperature may change dramatically. To accelerate code convergence, try changing the **[SCALE_OPT]** from **MAJOR** to **NONE** for a few iterations.

[INC_ADV] Include advection terms in the rate equations. These will generally become important when adiabatic cooling is important. Advection terms will be important when there are ionization changes in the wind, and when the flow time (R/V) is comparable to, or shorter than, the recombination time [$1/(\alpha Ne)$]. Essentially the same conditions for including adiabatic cooling.

[LIN_ADV] Hidden: compute advection terms using derivatives computed in the linear plane (default is TRUE).

[ADV_RELAX] Hidden: parameter to allow advection terms to be added slowly. Deafult is 1.0 (i.e., no scaling).

[INC_XRAYS] Include X-rays: Two choices are available: Pure- free-free emission can be chosen (which several underestimates the X-ray emissivity), or the X-ray emissivity be read from a data file which is output from the X-ray code of Raymond and Smith. At present only a table assuming solar abundances is available.

When X-rays are present, set **[MAX_CF]=1000** (.i.e., maximum continuum frequency= 1000 x 10^{15}Hz). This ensures that the frequency range is large enough to cover most of the auger ionization edges.

[FF_XRAYS] Assume X-rays arise from free-free processes only. If false, emissivities are read from table.

[X_SM_WIND] When clumping is switched on, there is an ambiguity in how to interpret the filling factors. When **[X_SM_WIND]** is FALSE, the clumped densities are used to evaluate the X-ray emissivity. When **[X_SM_WIND]**is TRUE, the emisisvity is multiplied by the clumping factor. In this case the X-ray emissivity will be preserved when Mdot/√f is held fixed.

[VS_XRAYS] X-ray smoothing width when SOB/CMF options are used.

[FIL_FAC_1] Filling factor for first X-ray component: $1.0\ 10^{-3}$. _2 denotes the second component. The X-ray emission is proportional to the square of the (local density) * (the filling factor). For very low mass-loss rates it may be necessary for the filling factor to exceed unity in order to match the observed X-ray luminosities.

[T_SHOCK_1] Shock temperature in program units of 10^4 K.

[V_SHOCK_1] Scale height in km s^{-1} indicating where shocks become important: Typically 400 km s^{-1}.

[XSLOW] When true, X-rays are included gradually in the MODEL. Its use is recommended when including X-rays in a previously converged model that did NOT contain X-rays. When TRUE, the X-ray filling factor (**[FIL_FAC_1]**) is first set to **[XFI1_BEG]**. After a suitable convergence of the model has been obtained, the filling factor is increased by a factor **[XSL_FAC]**. This process is continued until convergence, and should be done using **LAMBDA** iterations. This procedure is recommended since the populations of high ionization species can change by more than 20 orders of magnitude when X-rays are included. Ideally run the model for approximately 30 LAMBDA iterations to get convergence.

NB: The new version of CMFGEN automatically revises **[XFI1_BEG]** and **[XFI2_BEG]** in VADAT to the new revised values as currently being used in CMFGEN. If **[DO_LAMBDA_AUTO]=T** in **IN_ITS**, or if not set, CMFGEN will automatically switch to non-LAMBDA iterations when large changes have ceased, and **[FILL_FAC_1]** and **[FILL_FAC_2]** have reached their desired values.

[XFI1_BEG] Starting value for X-ray filling factor **[FILL_FAC_1]** when **[XSLOW**] is true. Try using a value like 1.0D-12, although the optimal value is model dependent.

[XFI2_BEG] As for **[XFI1_BEG]** but for the second X-ray component.

[XSCL_FAC] Factor to scale the X-ray filling factor by as the model converges. I typically adopt 100. If the scaled value is greater than **[FIL_FAC_1]** (or FIL_FAC_2), **[FILL_FAC_1]** is used.

[V_XRAY] Maximum velocity separation, in km/s, between evaluations of the X-ray photoionization cross-sections. Default if 0.5*VS_XRAYS.

Options for beginning a NEW model

[RD_IN_R_GRID] Read in a predetermined R grid? The file should have the same format as the departure coefficient files. Generally set to FALSE.

[LIN_INT] Linear interpolate populations from an ``old model.'' Should not be utilized when the stellar parameters have changed. Use the **[LIN_INT]** option when changing the atomic models, computation options, and the number of depth points. (If **[LIN_INT]** is TRUE, no temperature iteration is performed, and the temperature structure is read in).

[POP_SCALE] Scale pops to satisfy abundance equations. Usually TRUE, but can be useful if fudging start populations because model is having convergence difficulties.

[IT_ON_T] Iterate on the initial temperature distribution? Set to TRUE when initiating new model with *NEW stellar parameters*. If merely changing the atomic models, set to FALSE, and set **[LIN_INT]** to TRUE.

[T_INIT_TAU] When **[IT_ON_T]** is true, the temperature is initially set to an interactively determined temperature based on the electron density, and the temperature read in. This is only done for temperatures where the electron scattering optical depth is greater than **[T_INIT_TAU]**. Set to 2 for most models, and ideally value should be larger than **[GREY_TAU]**. The temperature computed with this method is subsequently revised using a grey model atmosphere.

[GREY_TAU] Set the temperature to its GREY value for $\tau >$ **[GREY_TAU]**, but leave the temperature unchanged in the outer wind. Typically adopt $\tau = 1$. For O stars with weak winds, 0.5 (or even a value of 0.1) is better. Lower values (i.e. around 0.1 to 0.3) work very well when T/TGREY is read in from GREY_SCL_FAC_IN (see below). This option is used to adjust the temperature distribution when initiating a new model.

It is now possible to read in a table of T/TGREY from another model from a file called **GREY_SCL_FAC_IN** (formerly GREY_SCL_FAC). This file should contain ND, and τ(Ross), T/T(gray) in two column format. **This is now the preferred option.** For current modeling, a file GREY_SCL_FACOUT is created which contains the relevant data in the appropriate format. For old converged models, the file, **GREY_SCL_FAC_IN**, can be created in DISPGEN by issuing the following sequence of commands: GREY, GR{e}, XROSS, T, TGREY, GR{VAR, /{1,2,3), WXY{GREY_SCL_FAC, 3} e}. You will need to edit out the first line of GREY_SCL_FAC (which contains the number of plots).

Option specifying method of handling lines.

[TRANS_DUM] Method for treating lines in species DUM. Available options are BLANK, SOB, and CMF. See description of **[GLOBAL_LINE]** option discussed above. These specifications are ignored **EXCEPT** if **[GLOBAL_LINE]=NONE.**

[DIE_AS_LINE] Treat dielectronic as non-overlapping lines. Preferred option is FALSE, particularly with blanketing calculations. The other option has not been tested recently, so **BEWARE.**

[VSM_DIE] Velocity (km s^{-1}) used to smooth dielectronic lines when added to photoionization cross-sections. Use a value similar to that used to smooth the photoionization cross-sections. The adopted value should **NOT** be less than **[V_CROSS].** Used to insure that aliasing doesn't occur when we sample the continuum photoionization cross-sections on a coarse frequency grid.

[DIE_XzV] Include Low Temperature Dielectronic recombination for species XzV. Two logical values must be specified. The first indicates whether normal dielectronic calculations are included. The second indicates whether dielectronic recombinations from levels forbidden to autoionize in LS coupling are included. The first must be FALSE when OPACITY photoionization cross-sections, which explicitly include the resonances, is utilized. **BE CAREFUL.**

Options for assisting convergence

[FIX_XzV] Fix the first **[FIX_XzV]** levels for species **XzV**. Option is mainly for debugging purposes. If a particular level is causing convergence difficulties, it cab be fixed while the other populations are solved for. Usually set to 0.

[FIX_DUM] To fix the highest available ionization state of species DUM, set to unity. For example, when DUM=HE, He^{++} is held fixed when all ionization stages of helium are included. Usually set to 0.

[FIX_NE] Fix the electron density. Option is mainly for debugging purposes. If the electron density is causing convergence difficulties, it can be held fixed when the other populations are solved for. Usually set to FALSE.

[FIX_IMP] Fix impurity species automatically. Option is mainly for debugging purposes. If a particular set of levels is causing convergence difficulties, and which have very low populations, they can be automatically held fixed when the other populations are solved for. Usually set to FALSE.

[FIX_T] Fix the electron temperature? Option is mainly for debugging purposes. If the Temperature is causing convergence difficulties, it can be held fixed when the other populations are solved for. Usually set to FALSE, although it can assist in difficult to converge models. This option is VERY useful. **It can also be used to compute models where the temperature structure is input, and is not to be changed.**

[FIX_T_AUTO] Allows the code to automatically hold the temperature fixed in the outer parts of the atmosphere to improve convergence reliability. The temperature is typically held fixed until the changes are less than a factor of 5. Normally set to TRUE. Setting to FASLE can speed up some models, but in most case it will lead to a more erratic convergence. Set to FALSE only if you know what you are doing.

[FIX_INB_T] Fix the inner boundary temperature at depth. Parameter is hidden with a default value of FALSE. It was installed to assist convergence of some time-dependent SN models with very large optical depths --- it should only be fixed when T has been set, at depth, to the grey temperature distribution, and the grey temperature distribution at depth is accurate. It should not be needed for stellar models. Used with **[FIX_X_DPTH]**.

[FIX_X_DPTH] Indicates the number of depths for which T is held fixed. It is only used when **[FIX_INB_T]=.TRUE.**

[TAU_SCL_T] Obsolete. Fix T for this optical depth. Normally set to 0. Useful for converging difficult models. **[FIX_T_AUTO]** is an automatic version of this option.

[T_MIN] Approximate minimum values that T can have in the converged model. Usually set to 0.0D0. Can be needed in some models because of exponential overflow s when computing LTE populations (i.e., when T=0.2 (i.e., 2000K) and you have FeX (for example) in the model.

[ADD_OPAC] Hidden: Experimental parameter. Adds additional opacity to model. Use for testing purposes ONLY. Unless you know what you are doing, this should be FALSE.

[OP_SCL_AFC] The added opacity has the form OP_SCL_FAC*SIGMA(THOMPSON)*N(ATOM).

[SOL_METH] Method for solving the LINEARIZE statistical equilibrium equations. Options are DIAG, TRIDIAG, and PENTADIAG. The NUM_BNDS variable in the MODEL_SPEC file must be compatible with the chosen option (i.e., can't choose TRIDIAG and have NUM_BNDS=1). NUM_BANDS=3 and the DIAG option is okay, except that it wastes memory. TRIDIAG is the best compromise between convergence and memory requirements. DIAG saves a factor of roughly 2 in memory, but converges much slower.

[SCALE_OPT] Option to indicate how the corrections found from the linearized statistical equilibrium equations are scaled, before they are used to improve the population estimates. Preferred option is MAJOR.

MAJOR At **EACH** depth the maximum change in any population is limited to a factor of **[MAX_LIM]**. All other corrections are scaled so that this is satisfied. Impurity species (i.e., those with very small populations) are not considered in determining the scaling factor. Their scaling factor is determined independently. For Λ --iterations the corrections are limited to a factor of **[MAX_LAM]**.

LOCAL As for MAJOR, but no distinction between impurity and major species.

GLOBAL As for local, but all depths are scaled by the same value. This option really slows convergence, and is never used!

NONE Scaling performed on each variable, without consideration of the corrections to other variables. Generally not recommended, but switching to this option can greatly accelerate convergence when the temperature needs large adjustments.

[EPS_TERM] Terminate model when maximum fractional change for a FULL linearization is < **[EPS_TERM]**%. Typically choose 0.1.

[MAX_LIM] Maximum factional correction to allow for a full linearization iteration. Thus an atomic population can be reduced by a factor of **[MAX_LIM]**, or increased by a factor of **[MAX_LIM]**. Typically adopt **[MAX_LIM]**=10. We use this limit to provide convergence stability.

[MAX_LAM] Maximum factional correction to allow for Λ iteration. Thus an atomic population can be reduced by a factor of **[MAX_LAM]**, or increased by a factor of **[MAX_LAM]**. Typically adopt **[MAX_LAM]**=10^5. For a new species, with very low abundance, this can be set as high as 10^{20}.

[MAX_CHNG] Terminate model with an error if the %fractional change is greater than **[MAX_CHNG]**. Typically we adopt 1.0D+10. A larger value is adopted when introducing a new species whose populations are very uncertain. Note that the POINT1, POINT2 and SCRTEMP files are still updated. Utilized as a warning that the model is likely to have difficulty converging.

[COMP_BA] Write the BA (the linearization) matrix out after each full iteration. Option normally set to FALSE. BA matrix will still be written out when MAXIMUM correction is less than **[BA_CHK_FAC]**.

[STORE_BA_INV] Store the inverse of the BA matrix. For very large matrices, this can save computational effort.

[N_FIX_BA] When the corrections are small. The BA matrix is held fixed (see **[BA_CHK_FAC]** option). To save even more time, we now can hold the BA matrix fixed for N_FIX_BA iterations, independent of the current correction sizes. The recommended value is 2.

[WRT_PRT_INV] Write out part of the inverse. Designed to save memory on system where the FULL BA matrix is larger than the available memory.

[STORE_BA] Write BA MATRIX out. Should be TRUE.

[BA_CHK_FAC] This option indicates when to hold the linearization matrix, BA, fixed. The BA matrix is written to the disk and used for subsequent iterations. Typically we adopt 5% for the largest fractional change. Option could be improved.

[LAM_VAL] When the largest fractional change (absolute value) is greater than **[LAM_VAL]**, a Λ-iteration is performed. Typically do a Λ–iteration if % change is greater than 400.

[NUM_LAM] Maximum number of Λ-iterations before a full iteration is again performed. Typically choose 2. Lambda iterations are performed to improve convergence.

Options for an enhanced spatial grid.

[INC_GRID] Allows an improved spatial grid to be created on which the radiative transfer equation can be solved. Useful for improving convergence in the presence of ionization fronts. Generally set to FALSE.

[ALL_FREQ] Use the improved spatial grid for all frequencies. Not used if **[INC_GRID]** is FALSE.

[ACC_END] Only use the improved spatial grid if the frequency (in units of 10^{15} Hz) is greater than **[ACC_END]**.

[N_INS] Number of points to be inserted into each interval of the depth grid. Extra points are only inserted between **[ST_INT]** and **[END_INT]**. No effect if **[INC_GRID]**=FALSE.

[ST_INT] Interpolate from **[ST_INT]** to **[END_INT]**. No effect if **[INC_GRID]**=FALSE.

[END_INT] Interpolate from **[ST_INT]** to **[END_INT]**. No effect if **[INC_GRID]**=FALSE.

[ND_QUAD] Use quadratic interpolation for ND-ND_QUAD to ND. Helps preserve diffusion approximation at depth. No effect if **[INC_GRID]**=FALSE. If > ND, it is set to 5.

[INTERP_TYPE] Type of interpolation for **[INC_GRID]** option. Use LOG or LIN. No effect if **[INC_GRID]**=FALSE.

Eddington and BA computation

[N_PAR] Rate at which BA matrix is updated by BA_PAR matrix. The BA_PAR matrix was included to help improve stability, as we UPDATE the BA matrix for every line, and for every frequency (although no problems were actually observed). BA is updated by BA_PAR every **[N_PAR]** frequencies in BLANKETING mode. Typically adopt ***2000***. NB: For small model 200 used to be the recommended value. However for large models, and LAMBDA iterations, this can significantly increase the required computation time.

[COMP_F] Tells **CMFGEN** whether to compute new Eddington factors. Generally set to FALSE. Simply deleting the EDDINGTON factor file can enforce this option.

[ACC_F] Accuracy with which Eddington factors are computed on each iteration. Typically we adopt 10^{-4}.

Parameters to control NG accelerations

[DO_NG] Do an NG acceleration when the maximum corrections are less than **[BEG_NG]**. An NG acceleration can be forced, after a model has completed, by running the FORTRAN program DO_NG, which reads the SCRTEMP file.

[BEG_NG] Typically choose 5% to 10%. Typically a model must run for over 10 to 15 iterations before an NG correction is applied, even if the corrections are small. When an NG acceleration is applied too early, convergence may be worse. A more sophisticated decision process for performing NG accelerations would help convergence.

[IBEG_NG] Even if the **[BEG_NG**] criterion is met, an NG acceleration is not performed until **[IBEG_NG]** iterations have been completed.

[BW_NG] Bandwidth (i.e., range of depths over which Ng acceleration is applied simultaneously). Used to use 1, but a value of ND may be better. NB: A value larger than ND is set to ND.

[ITS/NG] Number of iterations between NG accelerations. We typically adopt 8.

Auxiliary Programs

All executable names are lower case, end in .exe (i.e., cmf_flux.exe), and are located in $cmfdist/exe.

CMF_FLUX

Program to compute the spectrum in the Observer's frame. **This is the preferred method, and gives the most accurate observer's spectrum.** Results from this program are more accurate than those given in OBSFLUX (the output from CMFGEN) particularly for lines formed in the photosphere (e.g., most lines in O stars).

The full continuum spectrum, defined to treat all bound-free edges, is always computed. Using parameters defined in CMF_FLUX_PARAM_INIT, it is possible to limit the section in which lines are included, resulting in a considerable saving of computation time. A separate calculation must be done to compute the continuum flux at all wavelengths. This is handled automatically by **batobs.sh**.

Note that before the Observer's frame calculation is performed, 1 or 2 comoving frame calculations are carried out. In this section the emissivity and opacity are calculated. These will be transformed from the comoving-frame to the observer's frame in the observer's frame routine. In addition, this calculation allows the computation of the electron-scattering emissivity allowing for the frequency redistribution of line photons due to the thermal and bulk velocities of the electrons..

A variety of intrinsic absorption profiles can be adopted:

DOP_FIX: Doppler but with a fixed width. It is the same for all species and at all depths

Doppler: Variable --- uses correct atomic mass, and allows for a depth dependent turbulent velocity.

Stark: For H I and He II only. The approximate Stark profiles are convolved with a Doppler profile. They are generally adequate, except possibly for transitions between adjacent levels (e.g., Hα). Improved Stark profiles could easily be implemented.

Voigt At present, only radiative damping is included. LIST Profile options for individual lines are specified in the file FULL_STRK_LIST.

LIST_VGT This is the preferred option.
Use the options in FULL_STRK_LIST when available.
Uses a Doppler profile for "weak" lines.
Uses VOIGT profile with radiative damping for strong lines (those with a line to continuum ratio > 10^4).

Running CMF_FLUX

If the model was run in directory r1/, it is recommended that flux calculations be done in the directory r1/obs/.

The following files are required:

batobs.sh	Primary control file
CMF_FLUX_PARAMS_INIT	Basic control data. Key words that have a distinct meaning from those in VADAT are described later in this document. On some operating systems, you may need to make sure CMF_FLUX_PARAMS has been deleted before starting the job. NB: The parameters in CMF_FLUX_PARAM_INIT are generally independent of those in VADAT.
FULL_STRK_LIST	Contains type of intrinsic line absorption profiles to be used for individual lines if [GLOBAL_PROF] is set to LIST or LIST_VGT. Use the latest file in $cmfdist/misc/.
Atomic data files:	As used by CMFGEN. Assign using **batch.sh ass**. Taken care of by batobs.sh.
Output from CMFGEN:	MODEL RVTJ POPDUM (for all species)

Output from CMF_FLUX:

The following files are generated when the script batobs.sh is used:

obs_fin	Main spectrum. The file contains a list of frequencies (in 10^{15} Hz) and then lists the corresponding fluxes in Janskies (assuming d=1kpc). It is a raw data file --- no smoothing has been done and no effect of roation is taken into account.
obs_cont	Continuum spectrum (may contain dielectronic lines if they are treated as part of the photoionization cross-sections).
hydro_fin	As for CMFGEN. Values are only meaningful if the ENTIRE spectrum has been computed.
MEANOPAC	As for CMFGEN. Values are only meaningful if the ENTIRE spectrum has been computed.
OBSFLUX	If batobs.sh is used, this will contain the continuum spectrum as computed using

CMF_FLUX_OBS, and can be ignored. The full spectrum OBSFLUX file is copied to OBSFLUX_FULL batobs.sh. These files may be deleted.

Explanation of options in CMF_FLUX_PARAM

CMF_FLUX_PARAM is the main driver file for CMF_FLUX. Some parameters need to be included even when they are not utilized. A few parameters need only be included when another specific parameter has been set to a specific value.

All keywords in the following text are specified in bold between square brackets. Some parameters are checked for validity --- others are not. It is the responsibility of the user to ensure that the parameters are valid.

Keywords need not be in order, although it is recommended that the ordering of keywords not be changed from that provided. If a keyword can't be found, an error message is output to OUTGEN, and program execution stops. Superfluous keywords (e.g., PROF_CIII when CIII is not included) are ignored.

Additional keywords are continually added to improve the accuracy and applicability of the code. This will necessitate the CMF_FLUX_PARAM file to be to be revised, if you wish to re-compute an observer's frame spectrum. This generally presents no difficulty, however, since the options are unique, and the code will inform you through the OUT_FLUX file when they are not present.

Keywords that have the same meaning as in VADAT are NOT repeated here.

[NUM_ES] Number of iterations to be performed so that the incoherent electron scattering source function can be accurately computed. Set to 1 if **[COH_ES]**=TRUE. A value of 2 is generally found to be adequate. Higher values may give better accuracy, but increase computation time. On the fist pass coherent scattering is assumed.

[VTURB_FIX] Turbulent velocity in km s^{-1} at all depths. Only utilized If **[GLOBAL_PROF]**=DOP_FIX.

[VTURB_MIN] Minimum turbulent velocity in km s^{-1}. Utilized when **[GLOBAL_PROF]** .NE. DOP_FIX. The turbulent velocity is assumed to have the form

$$V_{TURB} = [\text{VTURB\_MIN}] + ([\text{VTURB\_MAX}] - [\text{VTURB\_MIN}]) * v(r)/V_{\infty}$$

[VTURB_MAX] Maximum turbulent velocity in km s^{-1}. Utilized when **[GLOBAL_PROF]** .NE. DOP_FIX.

[TAU_MAX] Integrations of the source function along a ray are truncated when τ exceeds **[TAU_MAX]**. 20 is a reasonable value.

[ES_TAU] Maximum step size for integrations on the Thompson electron scattering optical depth scale. 0.1 seems to work well in a variety of models. Higher values can be utilized with some models.

[INT_METH] Method for determining the intensity arising from a single ray. Two options are available:

ETAZ: Integral of the emissivity over *z*. Its advantage is that it can handle negative optical depths.

STAU: Integral of *S* over τ. Possibly the more accurate, but depends on choice of **[ES_TAU]**.

[WR_ETA] Write χ, χ_{es}, η, to direct access files, with the same format as EDDFACTOR. Can be plotted using PLT_JH. Also used by OBS_FRAME.

[WR_FLUX] Write H as a function of frequency and depth to a direct access file, with the same format as EDDFACTOR. Can be plotted using PLT_JH.

[WR_IP] Writes the outer boundary specific intensity, I, as a function of impact parameter p and frequency. File is a direct access file and can be plotted using PLT_IP. Still under development.

[WR_CMF_FORCE] Outputs the radiative line force computed in the CMF. The file has the same format as EDDFACTOR and gives the cumulative line force (starting in at short wavelengths) as a function of frequency. Use PLT_JH (specific options available) to display. This is only computed when **[BLANK]** is set to T.

[WR_SOB_FORCE] Outputs the radiative line force computed using the Sobolev force and the **unblanketed** continuum. The file has the same format as EDDFACTOR and gives the cumulative line force (starting in at short wavelengths) as a function of frequency. Use PLT_JH (specific options available) to display. This is only computed when **[BLANK]** is set to F (i.e., the continnum calculation) and **[DO_SOB_LINES]=T**. Because we use an unblanketed continuum, the force generally exceeds that computed in the CMF. It would be probably more realistic to smooth the continuum first.

[WR_ION_FORCE] Outputs the radiative line force computed in the CMF for each ion (bound-bound transitions only). The file (ION_LINE_FORCE) in ascii format, and is self explanatory. Due to non-linear interactions, the contribution by a given specified in ION_LINE force will not be identical to the change in line force that will occur when that species is removed. Only computed when **[BLANK]** is set to T.

[FRAC_DOP_OBS] Indicates the spacing, in Doppler widths, across the center of a line in the Observer's frame. Installed to allow more points across the photospheric profile in O stars. Has no effect if (effectively) larger than **[dV_OBS_PROF]**.

[GLOBAL_PROF] Indicates method for determining intrinsic line absorption profiles. Options are:

NONE Options for each species determined by **[PROF_XzV]**.
DOP_FIX Fixed Doppler width for all species.

DOPPLER Species and depth dependent variable Doppler width.
HZ_STARK Stark profile (convolved with Doppler profile) for H I and He II.
LIST Profile options for individual lines are specified in the file FULL_STRK_LIST.
LIST_VOIGT Use the option in FULL_STRK_LISt when available. Uses a Doppler profile for "weak" lines. Uses VOIGT profile with radiative damping for strong lines.

[PROF_XzV] Profile for individual ionization stage. Only utilized when **[GLOBAL_PROF]=NONE.**

[SCL_ABUND_DUM] Optional option to scale the abundance of an impurity species. Inserted to facilitate spectral analysis by allowing the effect of abundance changes to be quickly gauged. As a simple scaling may not be appropriate, **DO NOT** use this option for the final analysis. Instead you **MUST** use CMFGEN to compute a new model.

DISPGEN

Display package for examining the model atomic populations, plotting, test calculations etc. Routine requires MODEL, RVTJ, POPDUM files, and atomic data files. Options are discussed in **maingen_opt_desc.txt** and listed in **maingen_options.txt**. The help files can be made accessible to **DISPGEN** by issuing the shell script **astxt** in the run directory.

This routine is powerful, and easy to modify. Options are performed in MAINGEN. Using this package it is possible to:

Plot T, V, departure coefficients, populations, ionization fractions etc. versus a variety of parameters (e.g., log r/R_*, N_e, column density, depth etc.)

Compute approximate equivalents for individual transitions.

Compute net-radiative brackets, mean intensities etc.

A basic philosophy of DISPGEN is that it is OPTION driven. Each option passes data to **GRAMON_PGPLOT**, the plotting package, via a call to CURVE. The data is generally not plotted until the **GR** option (the default) is given. This allows many different curves to be placed on the same plot.

DISPGEN requires the atomic data files used by CMFGEN in computing the model. Soft links to the data files can be obtained by entering

batch.sh ass

where the batch.sh was the shell script used to run the model under consideration. The help files should also be assigned using **astxt** (this command could be placed in batch.sh).

DISPGEN will create a lot of files of the form
*.sve.
These are used so that an option can be repeated, e.g.,
.EW_CIV
will use the same parameters last used by the same option. In DISPGEN options must match EXACTLY. The shell command dsve will remove ALL files os the form *.sve .

In addition,
*.box
files can be created. These can contain a list of options (e.g., .EW_CIV) that are repeated in sequence. This is more useful with the PLT_SPEC program.

Commands beginning with x (e.g., xtemp) set the default X-axis but do not generate any plots. XTEMP, for example, sets the X-axis to temperature in units of 10^4K. Most other (y options) then use this as the default X-axis. A few options, because of their nature, use an alternate axis.

PLT_SPEC

Display package for plotting model and observed fluxes. Options are discussed in **pltspec_opt_desc.txt** and listed in **plt_spec_options.txt**. The help files can be made available to PLT_SPEC by issuing the shell script **astxt** in the current directory. This command should also be issued to make available the data for the interstellar lines.

The philosophy behind PLT_SPEC is similar to that behind DISPGEN except options can have extensions. Thus

RD_MOD
RD_MOD1
RD_MOD_T32

are all valid versions of the RD_MOD option, which allows model data to be input. Each will generate its own unique save file. Remember that the data in obs_fin (& OBSFLUX) assume d=1kpc, which is the default assumed by PLT_SPEC.

With PLT_SPEC it is possible to redden model data using a variety of extinction curves. It also possible to make a crude allowance for interstellar H and H_2, to apply a velocity shift, and to rectify data using a computed continuum. Further it is possible smooth the data to match the instrumental resolution, and to modify the observed spectrum for the effects of stellar roatation for a given **v sin i**. The philosophy behind PLT_SPEC is that model data is ``altered'' to match the observations —— the observed data is not altered.

The three most used options are RD_MOD, RD_OBS, and FLAM which are discussed below.

RD_MOD is used to read in model data (e.g., obs_fin or OBSFLUX). The X & Y axes will be determined by the XU (default is wavelength in Å) and YU (default is Jy) commands. RD_MOD immediately sends the data to the plot package (the assumed distance will be 1kpc) unless a hidden keyword (OVER) is set to T. If the model data is to be operated on, it must be read in with the OVER keyword set to true {i.e, RD_MOD(OVER=T) }. This will allow reddening corrections etc. to be done BEFORE the data is sent to the plot package. There is only one data buffer in PLT_SPEC --- the data can be easily read in repeatedly (if necessary) using the .RD_MOD option. Options which alter the data in the buffer include **ROT** (allow for rotation of the star), **ISABS** (apply H2 and H absorption by interstellar medium), **CNVLV** (smooth data). The **NORM** option can be used to divide the data by the continuum (obs_cont) in which case the default is to send the data in the buffer to the plot package. Alternatively the divided data can be saved in the buffer.

FLAM: Sends the data in the buffer to the plot package. At the same time reddening corrections, and a change in the assumed distance, is allowed for. The data in the buffer is not affected.

RD_OBS is used to read in observational data. Observational data is read in from text files in X,Y column format. As the default X is assumed to be the wavelength, and Y the flux. Data can also be read in when in multi-column format. The default is to send the data immediate to the plot package, although it can also be read in toe the data buffer by setting the hidden keyword MOD to

true (i.e., RD_OBS(MOD=T). At the top of each file several hidden keywords can be specified. These are used to indicate units, and whether the data is to be scaled.

The key word **FLUX_UNIT={}**is compulsory, and refers to the flux data in column 2.Comments can be listed at the top of the file before the keyword **FLUX_UNIT**. I suggest using ! to allow for possible format changes. Possible values for FLUX_UNIT are as follows:

FLUX_UNIT= {ergs/cm^2/s/Ang}
{egs/cm^2/s/Hz}
{mJy} {Jy} {Jansky}
{norm}.

In input the data is converted to Jy, but the **yu** command in PLT_SPEC allows the default y-axis to be changed. With the {norm} unit, no change is made. This is useful for reading in rectified data. **Xu** allows the x-axis unit to be changed.

Non compulsory key words:

WAVE_UNIT={Angstroms}{Micrometers{UM}{Hz}
AIR_UNIT ={TRUE}{FALSE}
Used to indicate whether wavelengths > 2000A are in air.
SCALE_FACTOR={Number}
Scale factor applied to the flux data.
FLUX_UNIT_n is used to refer to the data in column n.

Multiple data sets can be included in a single file. These MUST be separated by at least one row of '**********'. It must also have its own set of keywords which MUST begin with FLUX_UNIT=.

TLUSTY_VEL

Designed to allow you to used the hydrostatic structure from a TLUSTY run. To do this a file containing R, V and SIGMA (called RVSIG_COL for convenience) must be generated using **TLUSTY_VEL.EXE** (or some other program). The [VEL_LAW] is set to 7, [VEL_OPT] to RVSIG_COL, and [VINF] to the largest value in RVSIG_COL. The TLSUTY file *.11 (e.g., S40000g400v10.11) is required by **TLUSTY_VEL.EXE**. Basically a β-type velocity law is matched to the hydrostatic structure so that the velocity law, and its first derivative, are continuous. Ideally, this matching should be done around 1/3 to 1/2 times the sound speed.

Parameters needed for TLUSTY_VEL

R_*	Innermost radius of star(in R_{sun})
Rmax	Outer radius of star (in R_*).
Mdot	Mass loss rate (in M_{sun}/yr)
V_∞	Terminal velocity (in km/s). Depending on Rmax and β this value may slightly than the value in VADAT.
Beta_out	Value for β in outer wind -- β is the parameter in the classic velocity law $V_\infty(1-r/R_*)^\beta$.
Beta_in	Value for β in the inner wind. This was included to allow the wind velocity to be joined to the hydrostatic velocity law at velocities close to the sound speed (i.e., 1/3 to 1/2). Large β (>1) can yield a matching velocity of < 1km/s.
Beta Scale Height	Indicates how quickly to switch from the inner β to the outer β (in R_*).

The first 4 parameters must be consistent with those in VADAT. Usually we choose the inner most point to have an optical depth slightly less than 100. Three options can be used to determine the grid (which will be the grid used by CMFGEN). Basically one grid is adopted for the pgotpshere below 1 km s^{-1}, and a second grid is utilized above 1 km s^{-1}. The new default method appears to work well, and is recommended. It is a hard coded merged version of the other 2 options described below.

The two earlier methods are retained for compatibility; one is based on density, the other on optical depth. Neither worked too well in all cases. For O stars, I generally found that the best depth grid was created by combining the bottom 2/3 of one grid (ND=60) with the top 1/3 of the grid constructed with the alternate option (ND=60). This yield good coverage in velocity and optical depth at all locations in the atmosphere, with (typically) ND=67.

GRAMON_PGPLOT

Basic plotting subroutine which is option driven. Basic calling method can be seen in PLT_SPEC or DISPGEN. Package has a lot of options for making pretty plots. At present it does not allow multiple panels on the same page. This is not a limitation --- postscript files can easily be combined to give a panel format either by editing, or by running simple scripts (programs). **N_COL_MERGE.EXE** and N**_MULTI_MERGE.EXE** are two fortran programs designed to facilitate plot merging.
.sve files are not utilized by GRAMON_PGPLOT.

Data is passed to GRAMON_PGPLOT by calls of the form

```
CALL DP_CURVE(NPTS,XVEC,YVEC)
```

or similar variants. Up to 50 plots, of "arbitrary" length, can be passed. Error bars can also be passed. The plot package is called by

```
CALL GRAMON_PGPLOT(XLABEL,YLABEL,TITLE,OPTIONS)
```

All arguments are CHARACTER, and may be blank.

Basic philosophy is that plot package should provide reasonable default plots. These defaults can then be modified to make pretty plots. Once the user is a happy with a plot, it can be written to a hard file using the Z option. For pretty plots with strings, it advisable to set an explicit aspect ratio (the default aspect ratio is device dependent).

Plot options

H	Help
P	Plot graphs (default)
NOI	Leave data intact on exit (actually a switch). Default is to destroy data on exit. Make sure to cancel VEL option before issuing this command.
E	Exit from PLOT package
CL	Clear Graphics Screen
Z	Hardcopy (ZN=Asks for new hard device). Plots are automatically numbered as pgplot.ps pgplot_2.ps etc.

Axis and plot format

A	Define basic axis Parameters (Xstart, Xend etc)
2A	Define parameters for axis on right hand side.
F	Change default axis parameters
L	Modify Axis Labels and Titles
N	Change size of labels, tick marks, and plot borders. Set aspect ratio of plot.
LY	Switch between LINEAR/LOG Y axis labeling.
LXY	Switch between LINEAR/LOG labeling for X and Y axes

Line styles

B	Switch error bars on/off
C	Indicate how curves are to be connected
	L Normal line
	E Non-monotonic
	B Broken
	I Invisible
	V Vertical lines
	A Histogram - X vert
	H Histogram
CC	Change color settings
CP	Change pens (Color Index)
D	Switch dashed lines on/off
DE	Edit dashed lines one by one
W	Change thickness (line weights) of curves
WE	Edit line weights one by one
M	Switch marking of data points on/off
DC	Define a straight line continuum for EW
EW	Measure the EW or AREA of a single line in a plot. If continuum has not be previously defined, continuum is assumed to be normalized to unity.
GF	Fit a set of Gaussians (with an exponent not necessarily=2)to a section of normalized spectrum. The parameters of the Gaussian, and the EWs are output. Rerunning GF allows previous fit parameters to be used/edited.
DG	Draw the Gaussian fits (in black) (allows the plot screen to be cleared and updated.
MGF	Automatically fit a set of Gaussians to multiple plots. Start parameters are obtained either from a previous fit using GF, of from a file which list previous fits obtained using GF. Two results files, with different formats, are output.

Line and string options

VC	Define line vectors on the plot using cursor control.
VF	Read vector definitions from a file.
VE	Online edit of vectors (colors, size, location etc).
SC	Define strings on the plot using cursor control. String location is done by the numeric keypad (1 to 9).
SF	Read string definitions from a file.
SE	Online edit of strings (colors, size etc).

Data IO

WP	Write plots to a direct access file. Plots are labeled, and these labels are subsequently used byr RP to access the plot. This option and RP can be used to compare plots from different models. RUN DISPGEN in two windows, and use these options to transfer data between the programs. On program can open a null window for plotting.
WPF	As for WP but file name can be changed.
RP	Read plots from a (WP) direct access file. WP and RP are useful to transfer plots between different programs or models.
RPF	As for RP but file name can be changed.
WXY	Write a simple asci data file in column format
RXY	Read a simple data file that is in asci format.
SXY	Writes asci format in column format with id, I, and x(i), y(i) given sequentially for all plots.

Simple plot manipulation.

NM	Scale plot level to unity, or to match another plot.
VEL	Convert X axis to use km s^{-1}. Entering 0 will return you to the original input axis.
XAR	Simple X axis arithmetic with a constant (& Log, ALOG)
YAR	Simple Y axis arithmetic with a constant (& Log, ALOG)
VAR	Simple arithmetic on two plots.

History mechanism

OLF	Open file to log commands.
CLF	Close log file.
OIF	Open a previously generated log file for input. Cumbersome, as some commands can't be used in this mode, and previously issued commands can be important.
CIF	Return to terminal IO.

MAIN_LTE

Used to generate a table of Rosseland mean opacities. See README file, and examples, in $cmdist/lte_hydro. The opacity table is required by WIND_HYDR, and if using DO_HYDRO option in CMFGEN. One minor bug is that code can spend a long time iteratin on Ne if TMIN is set too low, and if the corresponding low ionization species are not included.

WIND_HYD

EIND_HYD is used to generate RVSIG_COL for use with a new CMFGEN mode. See README file, and examples, in $cmdist/lte_hydro. A table of Rosseland mean opacities must be supplied. The density structure is assumed to hydrostatic below the sonic point, and specified by the velocity law above the sonic point.

WR_F_TO_S

Generate file containing links between FULL and SUPER levels. The oscillator file is required as input. Can also read old F_TO_S link files. Old F_TO_S files can be edited by hand to create new super-levels. WR_F_TO_S can be used to clean these files so that super-levels are consecutively numbered. Unfortunately WR_F_TO_S does not currently operate on the interpolation column which is in a few F_TO_S files (e.g., He2_F_TO_S).

DO_NG_V2

Read in SCRTEMP file and do an NG acceleration. Useful when manually assisting a model to converge. SCRTEMP is automatically updated with the new population estimates. Various options are available.

NG	Perform an NG acceleration. Step size, bandwidth, and depths can be specified.
AV	Average the last 2 iterations. It is very useful if some populations are oscillating.
SOR	Applies the last set of corrections times SCALE_FAC. The maximum correction is limtied to BIG_FAC.
NSR	Applies the last set of corrections K times as a geometric series. That is X0=X1*(1+T)**K where T=(X1-X2)/X2
REP	Repeat the correction as defined by the last iteration, and a previous iteration (input by the user).
UNDO	Replace a set of depths by the previous iteration.

GUESS_DC

Allows new input files to be created with estimates of the departure coefficients. Requires an EDDFACTOR file with a previously computed radiation field, and all the atomic files need to be assigned (via batch.sh). For adding a new entire species, start with the lowest ionization stage first. This is now the preferred method for adding

additional atoms and species. After generating, it is recommend that USE_FIXED_J be set TRUE, and several LAMBDA iterations be performed. USE_FIXED_J should then be set FALSE, and EDDFACTOR/EDDFACTOR_INFO delete. This procedure is now handled automatically --- CMFGEN will revert to normal iterations once sufficient convergence has been achieved using USE_FIXED_J and normal LAMBDA iterations.

REWRITE_DC

Modify departure coefficient file to allow for level splitting. Primarily used to split individual LS levels into J states. Requires 2 oscillator files for use.

PLT_SCR

Plot data in SCRTEMP file, which contains the populations as a function of iteration. A variety of options are available to illustrate convergence.

PLT_RJ

Plot data (ie., J) in EDDFACTOR file and/or ES_J_CONV file. Partially superseded by PLT_JH.

PLT_JH

Plot data from a variety of scratch files created with CMFGEN and CMF_FLUX. Multiple files can be read in, using the RD_MOD option. Data files that cab be read include EDDFACTOR, ES_J_CONV, CHI_DATA, ETA_DATA, FLUX_DATA, CMF_FORCE_DATA, SOB_FORCE_DATA. Be careful with the y-axis label, which is not always correct.

PLT_IP

Plot data in IP_DATA file. The IP_DATA file contains the intensity data as a function of impact parameter and frequency. If can be created using CMF_FLUX.

LAND_COL_MERGE

Merge several LANDSCAPE pgplots together to make a single postscript file. The pgplot must have the correct size/aspect ration if merging is to look correct. Use CPS mode to create the figuers. **LAND_MULTI_MERGE** allows creation of multiple columns plots.

N_COL_MERGE

As for LAND_COL_MERGE but creates figures in PORTRAIT mode. Landscape mode is still used to generate the raw postscript files. **N_MULTI_MERGE** allows figures in multiple rows/columns to be created.

Atomic Data

All atomic data is stored in directories of the form

    something/ATOMIC/DUM/XzV/date

where date is of the form ddmmyy. Thus each species and each ion has its own directory associated with it. This storage method will facilitate updates, bookeeping, and transfer of files to collaborators. Several different data sets already exist for some species. Except for H/He, use the latest version. See the README file for possible comments. In some cases the data is from alternate source, and it is not obvious which is best. The compilation of the atomic data **is a nightmare. NB**. For the atomic data directories, we tend to use, I, II, III, IV etc instead of the usual CMFGEN conventions.

With care, the supplied atomic data is sufficiently accurate for computing the atmospheric structure, and for computing abundances. However, it is essential that users take time to understand the limitations of each atomic data set, particularly when determining abundances. In some cases, levels have been combined into a single level, and this may affect both the strength and location of some lines. Fortunately, the atomic structures have generally been chosen so that this is not a major issue. In other cases, line wavelengths are wrong because the observed energy levels and wavelengths are not known. For example, CMFGEN predicts the presence of Fe IV lines in the optical region of O stars. Unfortunately, **NONE** of the wavelengths for these transitions are accurately known. This can cause "spurious" features to appear in the spectrum. More importantly, it is possible that some of the FeIV lines could lie on top of other lines which are used for abundance diagnostics in the observed spectrum.

For each ionization file there are 4 principal data files that are required:

XzV_F_OSCDAT File containing energy levels and oscillator strengths. In the level list, only the columns containing the level name, statistical weight, oscillator strength and the ID number are important. In the line section, only the columns containing the f value, and the i-j column are important. For speed, the i-j column is used to assign the transitions to the internal array, not the level names. **The format of this file is important. Do note edit the file by hand, unless you know what you are doing.** To include additional transitions (e.g., intercombination lines) it is best to use **rewrite_osc_v2.exe.**

XzV_F_TO_S File containing information on which levels are going to be grouped together as a super-level. Use WR_F_TO_S to create. File can be edited by hand, and cleaned using WR_F_TO_S.

XzV_COL_DATA Table of collisional data.

PHOTXzV_A — Table of photoionization cross-sections for each level. Look at an existing file to see format. Tabulated data, and specific analytical expressions, are allowed. A indicates that the final state is the ground state n(actually super-level) of the next ionization stage.

PHOTXzV_B — As for PHOTXzV_A, but for photoionizations to an excited state. Not all species have such data. In many cases it is included directly into the A cross-sections.

DIEXzV — Contains a list of low temperature dielectronic recombination (LTDR) lines from the work of Nussbaumer and Storey. Be careful not to include the lines twice. Some of these lines are automatically included in the Opacity project photoionization cross-sections. File is not necessary if these transitions are not going to be included in the model.

Atomic data programs

A collection of programs to read various atomic data formats, and to write them out in a format suitable for CMFGEN is available. These programs are not well documented, and are somewhat messy. They can be made available on request.