

CMFGEN *MANUAL*

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Introduction

CMFGEN is a radiative transfer code designed to solve the radiative transfer and statistical equilibrium equations in plane-parallel or spherical geometry. It has been designed for applications to Wolf-Rayet (W-R) stars, O stars, Luminous Blue Variables (LBVs) and supernovae (SNe). For stars with stellar winds the mass-loss rate and velocity law (above the sonic point) must be specified — at present we cannot solve for them self-consistently. The hydrostatic structure, below the photosphere, can be determined 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. It is this mode that has been continuously used, and is the least likely to suffer from a problem due to an update in CMFGEN.

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

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.

It is possible to treat species in different modes simultaneously. This is primarily useful for flux calculations (done with CMF_FLUX). For example, a spectrum can be calculated showing only H I line transitions. Alternatively, a spectrum can be computed with all H I line transitions omitted. These two options provide a mechanism to determine the direct influence of a species on the spectrum.

Several different options/assumptions are available to compute the radiation field.

1. Solve the transfer equation for spherical geometry in the comoving-frame (default); this is the mode used when studying massive stars and their stellar winds.
2. Solve the static transfer equation in the plane parallel approximation.
3. Solve the transfer equation in the plane parallel approximation with a vertical velocity field (zero order in v/c).
4. Solve the static transfer code for a spherical atmosphere allowing for all relativistic terms.
5. Solve the time-dependent spherical transfer equation to first order in v/c for a Hubble flow.
6. Solve the time-dependent spherical transfer equation for all orders in v/c (still under development).

The last 3 options were primarily developed for work on supernovae.

References

- Busche, J., Hillier, D. J., 2005, AJ, 129, 454
Spectroscopic Effects of Rotation in Extended Stellar Atmospheres.
- Hillier, D. J., 2003, in *Stellar Atmosphere Modeling*, ASP. Conf. Ser., 288, 199, eds.
Hubeny, I. and Mihalas, D. and Werner, K., p. 199
On the Solution of the Statistical Equilibrium Equations.
- Hillier, D. J., Miller, D., 1999, ApJ, 519, 354
Constraints on the Evolution of Massive Stars through Spectral Analysis. I. The
WC5 Star HD165763.
- Hillier, D. J., Miller, D., 1998, ApJ, 496, 407
The treatment of non-LTE line blanketing in spherically expanding outflows.
- 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.
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Program Names

cmfgen_dev.exe	Main program to compute atmospheric structure.
cmf_flux.exe	Main program to compute observed spectrum.
dispgen.exe	General display and diagnostic package.
plt_spec.exe	Plot package to treat theoretical and observed spectra.
gramon_pgplot.f	General plotting package (called by other routines).

chk_phot.exe	Simple routine to check photoionization data file.
count_phot_data.exe	Count number of levels and data values in a photoionization file.
do_ng_v2.exe	Manual acceleration routine.
guess_dc.exe	Guess departure coefficients for a new model.
land_col_merge.exe	Merge postscript files into a single file (landscape format).
land_multi_merge.exe	Merge two postscript files into a single file (row/columns).
main_lte.exe	Compute Rosseland mean opacities.
mod_cool.exe	Creates summary of GENCOOL (heating./cooling rates).
mod_prrr.exe	Creates summary of PRRRXzV file (recombination/ionization) for a given species.
n_col_merge.exe	Merge N postscript files into a single file.
n_multi_merge.exe	Merge N postscript files into a single file (row/columns).
rev_rvsing.exe	Modify RVS_COL file. Can modify file for change in mass-loss rate, velocity law, number of depth points, grid spacing etc.
rev_rdinr.exe	Modify file (departure coefficient format) that can be used to define the R grid (RVS_COL cannot be in use). velocity law, number of depth points, grid spacing etc. Many options.
rewrite_dc.exe	Rewrite departure coefficient file.
rewrite_scr.exe	Rewrite SCRTEMP to reduce its size (default is final 2 iterations) or change its format.
set_new_sn_mod.exe	Changes SN associated options in VADAT file making it easier to go from time step 1 to 2. Can also be used for later time steps.
plt_dfr.exe	Plot the origin of the observed flux (as computed by cmf_flux.exe) as a function of depth.
plt_jh.exe	Plot J , H , χ , η etc from files with EDDFACTOR like formats. H , χ , and η files can be created by cmf_fluxe.exe
plt_jh_cur.exe	Similar to plt_jh.exe, but access the JH file produced for SN models.
plt_ip.exe	Plot/examine I as a function of impact parameter and frequency.
plt_phot_raw.exe	Plot cross-sections/check recombination data from photoionization file(s). Photoionization cross-sections can also be plotted in DISPGEN.
plt_scr.exe	Plot SCRTEMP file.
tlusty_vel.exe	Create a hydrostatic structure from a TLUSTY model.
wind_hyd.exe	Create a wind with a theoretical hydrostatic structure.
wr_f_to_s.exe	Create and modify links between levels and super levels

Species Names

Each atomic species has two abbreviations associated with it. These abbreviations are set in `cmfdist/new_main/mod/mod_cmfgn.f`. 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. 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. **In this documentation, DUM is used to refer to the species (e.g., CARB) while XzV refers to a particular ionization stage (e.g., C IV).**

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, X,
XI, XII, XIII, XIV, XV, XSIX, XSEV, X8, X9, and XX.**

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 have 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 used Sx for Si but there was still the possibility of confusion since SxI will conflict with SXI. The changeover is transparent to new users, but users with very old model 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 a species separator in DISPGEN commands. The separator could be changed in DISPGEN to something else (For example, 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 while 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. However, the “sve” filenames (which save the last used parameters for an option) are 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, default distance is 1 kpc.
Fluxes	Janskies: $1 \text{ Jy} = 10^{-23}$ ergs/ $\text{cm}^2/\text{sec}/\text{Hz}$ In OBSFLUX, fluxes assume $d=1$ kpc
Frequency	10^{15} Hz

Adopted solar values

Rsun	6.96×10^{10} cm	$[6.95508 \times 10^{10} \text{ cm}]$
Lsun	3.826×10^{33} erg s^{-1}	$[3.845 \times 10^{33} \text{ cm}]$
Teff(sun)	5784 K	$[5777 \text{ K } (5780 \text{ K})]$
Msun	1.989×10^{33} gm.	

The values in brackets are from AAQ(2000). An effective temperature of 5780 K is calculated from Rsun and Lsun.

Wavelengths: All plotting is done assuming vacuum wavelengths. Wavelength input can (generally) be for air (if $\lambda > 2000 \text{ \AA}$) or for vacuum. In the atomic data files, wavelengths are generally air for $\lambda > 2000 \text{ \AA}$; otherwise vacuum. Be careful — there is the potential for confusion. In CMFGEN itself, only frequencies are used, so there is no confusion.

Physical constants: Function calls (located in \$cmfdist/subs/phys_con.f) return cgs values.

Abundances: Solar abundances are taken from Allens Astrophysical Quantities by Cox (2000) p.29-31. For future reference, the adopted solar values are output to MOD_SUM. The abundances have not been updated to more recent estimates, since their values (particularly CNO) are still uncertain.

Main Variables

Variable	Description	Typical Value
ND	Number of depth points	50 to 100
NC	Number of core rays	10 to 15
NP	Number of rays (angles)	ND+NC
NUM_BNDS	Number of bands used for linearization	1 or 3
NCF_MAX	Maximum number 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	\leq NXzV_F
NXzV_IV	Number of important levels for ion XzV Only used in cmfgen_dev.exe	\leq 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 (super level) populations at each depth. It is the sum of the NXzV + number of atomic species + 2 (for T and Ne), and is computed by CMGEN.
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 fully 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, and is 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 may not be as clearcut as with NUM_BNDS=3, and Ng acceleration is an important tool for obtaining convergence. However, for SN models we routinely use NUM_BNDS=1, with great success.
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 cases 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. For SN modeling, we routinely use $ND=100$.

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 for 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. If an error occurs, keep increasing `MAX_SIM` until the error stops occurring.
9. The choice of `NXzV_F` (the number of levels in the model ion) is entirely up to the user (practical upper limit is set by the available atomic data). At present, only the first `NXzV_F` levels are used — that is, the levels must be contiguous in energy. This may mean the need for a very large atomic model if you want to include levels above the ionization limit. Reasonable choices are given in the supplied models. Further, it is relatively easy to test the influence of the number of levels on the model spectrum
10. `NXzV` (number of super levels) is also set by the user – its value must be consistent with the links specified in the `XzV_F_TO_S` file. Reasonable choices are given in the supplied models. It is important to realize that setting `NXzV` to `NXzV_F` is not necessarily the best choice (except for H and He), since it is likely that collisional processes are being underestimated, and these will tend to drive certain levels (e.g., those belonging to

the same LS state) into LTE with respect to each other. Further, increasing NXzV increases the memory requirements. The choice of NXzV can influence the observed spectrum.

11. For H, CNO, and Fe, the number of important levels (NXzV_IV) should be the same as the number of super levels (NXzV), especially when solving for the temperature structure of the atmosphere. For other elements, NXzV_IV can often be set to zero. The final 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 the temperature is not converging, or if some species give convergence difficulties, adjust the levels considered to be important. If in doubt, set NXzV_IV=NXzV. The inclusion of additional “IMPORTANT LEVELS” increases the memory requirement but gives the faster convergence. If you are holding the temperature fixed, the constraints on NXzV_IV are less stringent.

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`.

If you are a new user, check your installation by running some of the supplied models. If you are a regular user of CMFGEN, please run some of your existing models. With each new version, you may need to add additional keywords to the VADAT files. CMFGEN will report any missing keywords in OUTGEN — when it finds a missing keyword execution stops. While your calculations should yield models in “agreement” with older models, the agreement will not necessarily be exact because some code changes cause accuracy changes in the calculations. However, spectra computed using different versions of CMFGEN should agree closely — if there is a significant difference please report the difference to me. The more of these checks that are done, the less likely the chance that a new version will introduce an undetected bug.

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

$$NT \times NT \times (NUM_BNDS + 1) \times ND$$

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. Large models may require several Gigabytes of memory. When important levels are used, the memory is approximately

$$NT \times NILV \times (NUM_BNDS + 1) \times ND$$

floating point words.

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 $NSPEC \times NT \times (NUM_BNDS + 1) \times ND$.

In a very early version of CMFGEN, BA was 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 $NF \times ND^2$. 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 $NF \times NT \times ND$. 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. 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. NB. Due to excessive overheads, a call to TUNE should not be placed inside an innermost loop.

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 sense, 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 have found that 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 iterations. Further it is possible to simply average the last two iterations. After a manual Ng acceleration, CMFGEN should be restarted. For stability reasons, I strongly recommend that you perform a LAMBDA iteration when restarting the model. This can be done by setting both [DO_LAM_IT] and [DO_LAM_AUTO] to TRUE in IN_ITS before restarting the model.

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. A 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_cmfgn.sh. 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. On some

systems and for some model regimes, it may be more efficient not to write the *SCRATCH* files — this is set by a parameter in VADAT.

Convergence

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

Λ -iteration,
full linearization,
full linearization,
hydrostatic density correction,
 Λ -iteration,
full linearization,
full linearization,
Ng Acceleration,
 Λ -iteration,
full linearization,

constitutes 10 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 20. 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 30 or more 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

$$r = (\text{previous correction}) / (\text{current correction}) = b/a$$

an estimate of the true error is $a/r + a/r^2 + a/r^3 \dots$ which is approximately $a/(r - 1)$. 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 (and with a truly converged model). When using the tridiagonal operator, it is relatively easy (but not generally 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:

1. 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. These instabilities occur, for example, in some LBV-like models.
2. 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, as can adding additional grid points in the neighborhood of the discontinuity.

3. A few levels at one depth (or a few depths) have very bad population estimates. Successive iterations do not 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, or with DISPGEN, will assist in obtaining convergence. Including additional depth points at the region of instability may also improve convergence.
4. The temperature structure is not converging. If you are using `cmfgen_dev.exe` with levels omitted from the full linearization (i.e., `NXzV_IV < NXzV`) the inclusion of additional levels (usually for the most abundant species) will help the convergence. Alternatively, you may need to increase the number of super levels,
5. You are using a diagonal operator, which has an inherently slower asymptotic convergence than the tridiagonal operator.
6. A few populations at a few depths are oscillating and show larger corrections than other populations (as seen in `CORRECTION_SUM`). You can use `ADJUST_CORRECTIONS` and/or `DO_NG_V2.EXE` (see page 40).

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 will inform users of important bugs — eventually there will be 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.

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 and tested in BLANKETING mode.
- 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 to adjust T at a range of depths, and recompute new departure coefficients assuming the populations are held fixed.
- 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 bugs

- One of the lower levels in the N I data has the wrong statistical weight. I will fix this as soon as I get a chance. It is not a simple change, since the f values to the state may change (depending on where they come from etc).
- In some atomic modes, a few levels have the wrong energy order (the levels have virtually identical energies). This will make no difference, provided you do not end the model atom with one of these levels.
- Some line wavelengths are inaccurate. Due to the coupling with the atomic levels, and adopted atomic data, these are not necessarily easily fixed. When computing spectra using CMF_FLUX, revised wavelengths for important lines can be specified in the file \$cmfdist/misc/REVISED.LAMBDAS.
- The Ar v data set \$ATOMIC/ARG/V/1dec99/fin_osc should not be used. Use instead \$ATOMIC/ARG/V/1dec99/arvosc_rev.dat (as stated in the README file). If the Ar v line at 1345Å is too strong, make sure you are using the correct data set. As a precaution, you might like to rename the fin_osc file in the atomic data set so you don't accidentally use it — I ship it to maintain compatibility for testing etc.

Installation

For installation purposes it is recommended that you adopt the same directory structure used by the author. This will automatically be obtained when you untar the distribution package. After untaring, it is suggested that you move CMFGEN into a distribution directory of the form

[cmfgen/date/](#)

(or some similar variant) where “date” refers to the current distribution date. In the following this distribution directory will be referred to as `$cmfdist`. 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, bookkeeping, and transfer of files to collaborators. Several different data sets already exist for some species. It is a nightmare. NB. For the atomic data directories, we tend to use I, II, III, IV etc. instead of the usual CMFGEN conventions.

You should also place the following (or equivalent) command in the shell source startup file (e.g., `.tcshrc` for the `tc-shell`).

[source \\$cmfdist/com/aliases_for_cmfgen.sh.](#)

where `$cmfdist` must be expanded to its full path. This defines the source directory (`$cmfdist` or `$CMFDIST`) and atomic data directory (`$atomic` or `$ATOMIC`) for the shell. The `cmfgen` script also defines command names for common programs (e.g., `cmfgen` for `$cmfdist/exe/-cmfgen_dev.exe`, `plt_spec`, `dispgen` etc), and well as other useful commands (page 30). Users should check that the `cmfgen` scripts do not conflict with their own scripts.

External routines/packages required by CMFGEN

PGPLOT

Free package available off the WEB (see <http://www.astro.caltech.edu/~tjp/pgplot/>). Used by many of my routines for line drawings. I have a MAC version on my website.

BLAS

Basic procedures for performing matrix manipulations. Should be available with the F90 compiler. If not, generic FORTRAN routines (obtained off the web) are supplied, but these will be less efficient than the system dependent BLAS routines. The compiled generic routines are placed in `lib/libmy_blas.a`. The `my` was inserted to avoid using these libraries inadvertently.

LAPACK FORTRAN numerical library

Often comes with F90 compiler. If not, routines available on the WEB. Several are supplied. The compiled routines are placed in `lib/libmy_lpack.a`.

Makefile

The distribution comes with Makefiles which will allow compilation of CMFGEN on your UNIX system. I have been successfully using the standard make on Mac and Linux systems. 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 for pgplot, blas, lapack, etc are correct.

Then

```
make clean
```

which removes all object files, libraries, executables from the distribution directories

Then

```
make i >& HOPE
```

does 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 \$cmfdist/exe will contain the following files (plus many others):

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.

NB: All file dependencies should be specified in the Makefile. However, I have been known to miss some of them. If strange errors occur, after updating a subroutine (particularly modules), the user should recompile and link all routines.

Makefile System Dependencies

Redhat 6.1 Supplied Makefiles work moderately well, with only a few minor (and insignificant) problems. Over the last few years I have only used them in LINUX systems, and on an Intel MAC.

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 \$cmfdist):

```
set MAKELIST='find . name Makefile' tar cvf linux_make.tar $MAKELIST
```

Possible Compilation Problems

1. New compiler releases (especially major updates) often contain bugs which are fixed in subsequent revisions. Thus I highly recommend not deleting your current FORTRAN compiler (especially if it works) when a new version comes in.
2. Most of the programs and subroutines 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.
3. Some compilers may insist on certain file extensions. A HP compiler will not compile programs of the form *.for. The usual convention on most compilers is that compilers assume *.f to contain formatted fortran files, while *.f90 files are unformatted.
4. Several programs (e.g., CMFGEN, CMF_FLUX, DISPGEN) use modules for data storage. In these modules, data types are defined. For example, mod_cmfgn.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 behavior and structure of CMFGEN and its routines is independent of which declaration is used.
5. For historical reasons most routines use the notation **REAL*8**. Most compilers have switches to change/override this. On alphas, with the PGF 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 the exception of routines in the pgplt directory (discussed below). All programs can be compiled to use the default INTEGER size (but at least 4 bytes).

The only routines that uses REAL*4 are routines related to PGPLOT since pgplot uses REAL*4. – The data storage module for the plotting routines, MOD_CURVE_DATA, also uses REAL*4 to save space. This is done simply to conserve memory. Data to GRAMON_PGPLOT is generally passed as REAL*8 via DP_CURVE. A few routines don't use the REAL*8 notation, but this should be taken care of in the Makefile.

6. 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.
7. 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 it is not interpreted as a control character.
8. 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 ...
9. On some compilers, \$cmfdist/disp/maingen.f can take a long time to compile. If this occurs, change \$cmfdist/disp/Makefile so that maingen.f compiles with a lower level of optimization. It will not noticeably effect performance of this interactive program.
10. 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.
11. Routines with known system dependencies are placed in \$cmfdist/unix, and may need to be edited. The main routines that may need editing are **tune.f**, **date_time.f**, and **set_line_buffering.f**. The default routines work under pgf fortran with MAC and LINUX systems. With Intel compilers **set_line_buffering.f** should be changed to a dummy routine — it is used to stop buffering of ASCII files with pgf. No buffering is the default with Intel systems.
12. The Intel Compiler can have issues, and these change from release to release. I used


```
FG = -cm -extend_source -w95 -w90 -nbs -O3 -axTW -I$(MOD_DIR)
```

 when compiling. In the latest release (at least on a Mac Pro) you may need to change the Makefiles to force some modules to be linked. The latest INTEL compiler would not link pure modules that were in Libraries. It did not run successfully with OMP.

Run time problems

1. With some Intel compilers, some character statements are incorrectly handled. When this error occurs CMFGEN stops almost immediately, complaining about missing data files. The two most likely occurrences arise in [\\$cmfdist/newsups/genosc_v8.f](#) and [\\$cmfdist/newsups/rdphot_gen_v2.f](#). To fix the error do the following: In the first routine change FILNAME to have an explicit length “LEN=20”, while in the second change DESC to have an explicit length “LEN=12”, and recompile.
2. You have compiled the code using INTEL with parallelization, and it crashes in the `$cmfdist/plane/fg-j_cmf_v12.f` routine. This seems to be a bug with the INTEL compiler. Simplest fix is to comment out the OMP parallelization statements in `fg-j_cmf_v12.f`.
3. You have compiled the code using GFORTRAN.

Parallelization

Some of the routines associated with `cmfgen_dev.exe`, `cmf_flux_v5.exe`, and `main_lte.exe` have been parallelized using OMP commands. To implement the commands in the executable, compile/link options need to be specified. For the pgf95 compiler, for example, I define F90 as `pgf95 -mp`. These commands significantly improve the execution of the code on systems with multiple processors (e.g., factor of 2 to 3 faster with 4 processors). Using more than 8 processors does not lead to significant gains.

These parallelized routines work under pgf version `pgi/osx86-64/10.8/bin/pgf95` on a MAC, and pgf version `linux86-64/10.5/bin/pgf95` on LINUX AMD systems. Later versions should also work — I simply have not updated my compilers. I have had trouble with some routines (e.g., `$cmfdist/plane/fg-j_cmf_v12.f`) with the Intel compiler. OMP instructions can be removed from individual routines by adding an additional `!` to the line containing the OMP command.

I recommend users first installing CMFGEN without parallelization. If that works, then install a parallelized version. Compilers seem to have much more difficulty (i.e., they have more bugs) with parallelization.

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. The *.INC files MUST be upper case. The current version is stored in \$cmfdist/

main

No longer used.

new_main

Contains the main program and Fortran include files for main program. Most .INC files have been converted to subroutines.

cmfgen.f	Main Calling routine
cmfgen.sub.f	Workhorse
GET_J_CHI.INC	

new_main/mod_subs

Contains module definitions for use with cmfgen. At present two versions of mod_cmfgen.f are supplied. The default uses the new fortran structure which allows allocatable arrays to be used in structures. Some compiler versions (e.g., old intel) did not yet allow this option, so use mod_cmfgen.f.intel (although it has not be utilized for some time). No other changes to the code are required.

new_main/subs

New subroutines. Kept in this location for simplicity.

new_main/subs/auto

Routines to handle autoionization.

new_main/subs/chg

Routines handling charge exchange.

new_main/subs/non_therm

Routines handling non-thermal ionization and excitation.

new_main/subs/two

Routines handling two-photon processes for H and He.

com

Contains simple scripts to facilitate running models etc.

disp

Contains DISPGEN display package.

disp/subs

Auxiliary subroutines for DISPGEN.

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 (it has not been updated/tested for ages), and requires J, η , and χ 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.

plane

Originally contained subroutines for undertaking radiative transfer in plane-parallel geometry. It now also contains relativistic and time dependent radiative transfer routines, and updated versions of my main transfer routines.

spec_plt

Contains routines for displaying theoretical and model spectra (plt_spec), moments of the radiation field (plt_jh; plt_jh_cur), intensity data (plt_ip), flux origin (plt_dfr), and populations as a function of iteration (plt_scr).

spec_plt/subs

Auxiliary subroutines for PLT_SPEC.

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.

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, bookkeeping, 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 associated with each ionization stage for possible comments. In some cases the data is from an 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 Fe IV lines could lie on top of other lines which are used for abundance diagnostics in the observed spectrum.

For each ionization stage there are 4 to 6 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. A -ve ID indicates that the energy of the level has not been determined experimentally (and hence can be regarded as unknown) – in most cases, but not all, this is reliable. 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 NOT 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 (often a super level linking levels in the lowest term) 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.

AUTO_XzV_DATA

Contains list of autoionization level probabilities for levels above the ionization continuum.

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.

Useful Scripts

Several useful scripts can be found in the \$cmfdist.com directory. To use these scripts:

1. Edit the file /com/aliases_for_cmfggen.sh. Replace all occurrences of hillier (or jdih) 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.
2. Put the command

```
source /dist/com/aliases_for_cmfggen.sh
```

in your .tcshrc file. You will need to source the file — afterwards this will be done automatically when you login. The aliases_for_cmfggen.sh defines 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 are satisfied with the convergence of the model. You may want to remove the deletion of the EDDFACTOR and EDDFACTOR.INFO files from the command, as this file is sometimes useful when starting other models. To recover a deleted EDDFACTOR file you will need to do a single iteration.

NB: I tend not to remove the SCRTEMP and POINT files, since these make it easy to run additional iterations in the same directory. However, the commands \$cmfdist/exe/rewrite_scr.exe and \$cmfdist/com/mvscr.sh can be used to generate a smaller version of SCRTEMP containing only the last N (default is 2) iterations.

rmlinks Removes soft links. This option 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 in all lower directories.

rmin Removes all files of the form *_IN (no prompt)

rmrrr Removes all files of the form *PRRR (no prompt)

dfort Removes all files of the form fort.* (no prompt)

dlog Removes all files of the form *.log (no prompt)

dscratch Removes all files of the form *SCRATCH* (no prompt)

dsve Removes all files of the form *.sve (no prompt)

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 Compares ALL *.f, *.sh, *.INC and Makefile files in one directory with those in another. If only one directory is supplied as a parameter, the current directory is assumed to be the primary directory. To compare the current distribution with the previous distribution do the following in \$cmfdist:

```
$cmfdist/com/full_diff.sh $old_cmfdist > Error
```

or

```
$cmfdist/com/full_diff.sh $old_cmfdist >& Error
```

In the first case error messages related to files for which there are no counterparts in the old distribution directory is written to the screen, while in the second case they are written to “Error”. Error will also congaing other information about the directories examined etc. The file [Diff_sum](#) will list all examined files, and show differences when they occur.

for_diff Compares ALL *.f files in one directory with those in another. If only one directory is supplied as a parameter, the current directory is assumed to be the primary directory.

INC_diff Compares ALL *.INC files in one directory with those in another. If only one 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 5 primary control files:

- batch.sh** Controls model execution, and creates soft links to the atomic data.
- HYDRO_DEFAULTS** Only needed when a hydrostatic iteration is to be done.
- IN_ITS** Contains the maximum number of iterations to be attempted, and can also be used to force Λ -iterations.
- 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.

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, all the required input data files (discussed below) need to be copied to the directory of the new model. The simplest method of doing this is as follows:

```
cpmod r1 r2
```

In the above **r1** is the old model directory and **r2** is the new model directory. If **r2** is the same as **r1**, you will be requested to confirm the command. The above command does the following:

```
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
```

It also renames the *OUT files to *_IN by issuing the command

```
out2in
```

If they exist, the following files are also copied.

```
cp r1/RVSIG_COL      r2/
cp r1/HYDRO_DEFAULTS r2/
cp r1/ROSSELAND_LTE_TAB r2/
```

If the directory **r1** contains JH_AT_OLD_TIME, the model is assumed to be for a supernovae and the following additional files (JH_AT_OLD_TIME, JH_AT_OLD_TIME.INFO, NUCLEAR_DECAY_DATA, OLD_MODEL_DATA, & SN_HYDRO_DATA) are also copied. **The cpmod command should not be used to generate input data for a new SN model in a SN time sequence (use drad_cpmod instead)** — it is simply used to allow a revised SN model to be run at the same time step as the existing model.

In general, running a model requires the following steps to be performed. NB: It is not necessary to perform all of these steps for every model. For example, suppose you are computing a small grid of O star models, and you already have one model computed. Since MODEL_SPEC and batch.sh have already been edited, you may skip steps (1) & (2). If the abundances are also fixed you can skip step (7)— it is also probably reasonable to skip this step if you are not changing the abundances of the most important species.

1. 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 continuing an existing model, the populations will be obtained from SCRTEMP — you do not need to update the XzV_IN files.

2. Edit the batch.sh file so it points to the appropriate directories. On a Unix system soft-links (**ln -sf**) are used to point to atomic data files.
3. 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 Ar III has been deleted from the MODEL_SPEC file, it is not necessary to delete all occurrences of Ar III (e.g., FIX_ARIII) from the VADAT file.
4. 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.
5. If running a hydrostatic model, you may need to update RVSIG_COL using \$cmfdist/-exe/rev_rvsig.exe. An update is needed if you change the mass-loss rate, if you change the core radius of the star, if you change the velocity law, or if you change the number of depth points. A change is not needed for a change in abundances, a change in $\log g$, a change in model atoms, or a change in which species that are included. A RVSIG_COL file can be created from scratch using \$cmfdist/exe/tlusty_vel.exe, \$cmfdist/exe/wind_hyd.exe, or from an old model using DISPGEN.
6. If running a hydrostatic model, edit HYDRO_DEFAULTS to indicate the required number of iterations — this number decreases as the model runs. It may be altered when the program is running.
7. If the abundances of important species have changed, if you have changed the turbulent velocity, or have significantly changed the model atoms and species, you may need to update ROSSELAND_LTE_TAB.
8. 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 iteration (stored in SCRTEMP) to restart.

Some specialized cases for starting a new model are discussed below. These examples assume that the command

`cpmod r1 r2`

has been issued, and that you reside in the **r2** directory. It also assumes `$cmfdist` and `$atomic` are correctly defined via `aliases_for_cmfdgen.sh`.

Case 1: Running a supplied model

Use the `cpmod` command to copy the required model files into the new model directory, **r1**. Edit IN_ITS to set the number of iterations, and set `[LIN_INT]=T` in the VADAT file. Start the model by issuing `batch.sh &`. If the model crashes (or stops quickly), see if OUTGEN has been created. If it has, check the bottom of OUTGEN to see any error messages. The most likely error is that you will need to add a new keyword (or keywords) to VADAT. If it has not been created, see the compilation section for possible causes.az

Case 2: Change in number of depth points.

You wish to run a model which only differs from **r1** in the number of depth points. Use the `cpmod` command to copy the required files from **r1** to **r2**. Before starting the model you need to edit two lines in MODEL_SPEC (those containing ND and NP). In the VADAT file, set `[LIN_INT]=T`. If using the RVSIG_COL file, you will need to run REV_RVSIG to update the number of grid points. You MUST also set the number of hydrostatic iterations in HYDRO_DEFAULTS if you wish to update the hydrostatic structure.

Case 3: Changing abundances

You wish to run a model which only differs from **r1** in the abundances. Use the `cpmod` command to copy the required files from **r1** to **r2**. In the VADAT file, set the new abundances, `[LIN_INT]=F` and `[IT_ON_T]=T`. For the abundances, I recommend using mass fractions for all elements more massive than oxygen. If you do this, changes in the H/He ratio etc. will not cause abundance changes of iron group elements whose mass fraction is independent of changes in the H, He and CNO abundances. Edit IN_ITS to set the number of iterations. Depending on the size changes, you may, or may not wish to set `[DO_LAM_IT]=T`, `[DO_LAM_AUTO]=T` and `[DO_T_AUTO]=T` in IN_ITS, and `[FIX_T]=T` in VADAT.

If utilizing the `[DO_HYDRO]` option, you may need to compute a create a new ROSSELAND_LTE_TAB file. This file does not affect the solution — it only aides in converging the hydrostatic structure. Experience suggests that updating this file is probably not necessary if you are changing only the CNO and other metal abundances. If the model has difficulty converging the hydrostatic structure, update the file! Updates will be more necessary when you are close to the Eddington limit since these models are intrinsically difficult to converge.

Case 4: Revising the number of super-levels or changing the atomic model.

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**. Use the `cpmod` command to copy the required files from **r1** to **r2**. Edit the `MODEL_SPEC` file to reflect the changes, and set `[LIN_INT]` to true in `VADAT`. If using alternative data, or changing the association of super-levels with full-levels, you may need to change the atomic data assignments in `batch.sh`. Edit `IN_ITS` to set the number of iterations. In general, and particularly if you are including many additional levels and/or making considerable changes to the model atom, you should set `[DO_LAM_IT]=T`, `[DO_LAM_AUTO]=T` and `[DO_T_AUTO]=T` in `IN_ITS`, and `[FIX_T]=T` in `VADAT`.

Case 5: Revising $\log g$

You wish to revise the gravity of an existing model (which has an associated `RVSIG.COL` file). Change the gravity in the `VADAT` file, and set the number of hydrostatic iterations in `HYDRO.DEFAULTS`. The gravity is only utilized when a hydrostatic iteration is performed. Be careful — simply changing “ $\log g$ ” in `VADAT` will **NOT** change the hydrostatic structure. **When starting the model do not forget to edit `HYDRO.DEFAULTS` to indicate the number of hydrostatic iterations to be performed – as it was copied from a previous model the number of iterations to be performed will most likely be set to zero.** An error is output to `OUTGEN` when `[DO_HYDRO]=T` in `VADAT`, and when the maximum error in the hydrostatic structure is greater than 20% (at any depth), or if the root mean square error is greater than 5%. The star’s `MASS` in `VADAT` does not need to be changed — this will be updated by `CMFGEN`. When starting the model, you can use `[LIN_INT]=T`.

Case 6: Use `TLUSTY` hydrostatic structure

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 `[VIN]` to the largest value in `RVSIG.COL`. The `TLUSTY` file `*.11` (e.g., `S40000g400v10.11`) is required by `TLUSTY_VEL.EXE`. A program (`$cmfdist/exe/-rev_rvsig.exe`) can be used to revise `RVSIG.COL` (e.g., to change number of grid points, mass loss rate, velocity law etc.).

Case 7: Changing L , R_* , or \dot{M}

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 and change `[LIN_INT]` to `.FALSE..`

A file (`GREY_SCL_FAC_IN`), taken from model **r1**, contains $T/T(\text{grey})$ as a function of Rosseland optical depth. When present, this is used to scale $T(\text{grey})$ so as to provide a better estimate of the temperature structure. This is found to give a significantly better flux conservation at the beginning of an iteration. `GREY_SCL_FAC_IN` is obtained from `GREY_SCL_FACOUT` (see the `GREY_TAU` option description in `VADAT` description for more details), and is generally created by the `cpmod` command.

Experience suggests that starting with Λ -iterations provides greater stability. Thus set `[DO_LAM_IT]=T` and `[DO_LAM_AUTO]=T` in `IN_ITS`. The `IN_ITS` file will be updated by `CMFGEN` to have `[DO_LAM_IT]=F` once sufficient `LAMBDA` iterations have been done.

Experience also suggests that holding T fixed for the earlier iterations often provides greater stability, particularly if using `GREY_SCL_FAC_IN`. Thus I recommend keeping `[FIX_T]`

=T in the VADAT file, and set [DO_AUTO_T]=T in IN_ITS (NB: default is F). When this is done, initial iterations have T held fixed. Only when the corrections are “small”, will T be allowed to vary. The VADAT file will be updated by CMFGEN so that it now contains [FIX_T]=F. No manual intervention is required.

NB: If you are using the hydrostatic option (rather than a fixed velocity law in both the wind and photosphere) you will need to revise RVSIG_COL using \$cmfdist/exe/rev_rvsig.exe to reflect the new values. For example, suppose you just change \dot{M} . Only the density structure of the wind will change – the density structure below the photosphere will be fixed. The program \$cmfdist/exe/rev_rvsig.exe adjusts $V(r)$ in the photosphere to keep the density constant. A transition velocity (e.g., 10km/s) to describe the switch from photosphere to wind is requested .

Case 8: Revising T_{eff}

You wish to revise the effective temperature, leaving the gravity fixed. This a little more complicated, especially if you want to leave the V magnitude fixed. If you are not worried about the V magnitude, then simply adjust the Luminosity according to

$$L(\text{new}) = L(\text{old}) [T_{\text{eff}}(\text{new})/T_{\text{eff}}(\text{old})]^4 .$$

For exploration runs this is fine — photospheric O star spectra are sensitive to $\log g$ and T_{eff} only – they are very insensitive to the physical size of the star. \dot{M} might need to be scaled slightly to preserve line EWs.

If you wish to preserve the V flux (at least approximately) you will need to scale the radius. I use a simple little program to compute

$$R_*(\text{new}) = [B(\text{old})/B(\text{new})]^{0.5} R_*(\text{old})$$

(assuming $F(V) = \text{constant } B(T_{\text{eff}}).R_*^2$), and compute the luminosity from

$$L(\text{new}) = L(\text{old}) \left(\frac{T_{\text{eff}}(\text{new})}{T_{\text{eff}}(\text{old})} \right)^4 \left(\frac{R_*(\text{new})}{R_*(\text{old})} \right)^2 .$$

Due to the assumption regarding the scaling of $F(V)$, and since the relationship between R_* and $R(\tau = 2/3)$ will change slightly, this procedure is only approximate. You will need to revise RVSIG_COL using \$cmfdist/exe/rev_rvsig.exe to reflect the new value of R_* .

In both cases you need to set the number of hydrostatic iterations in HYDRO_DEFAULTS, and set [LIN_INT]=F in VADAT.

NB: Three stellar parameters can be specified in VADAT: L , R_* , and T_{eff} . These are not independent! For non-hydrostatic models (i.e., when DO_HYDRO=F [or is not present] L and R_* are used to define the model. T_{eff} is not utilized, and the value you have specified in the VADAT file may be far from reality. When DO_HYDRO=T, and you remember to actually perform hydro-iterations), L and T_{eff} are used to define the model. R_* will be updated to reflect changes in the hydrostatic structure below the photosphere. Also note for historical reasons, R_* is the radius of the star at the inner boundary – it is NOT $R(\tau = 2/3)$. This can be obtained from L and T_{eff} , and will be given in the MODEL_SUM file.

Case 9: Include additional ion(s)

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. NB: `CMFGEN` will stop, writing an error message to `OUTGEN`, if a required key-word is missing.

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

Preferred Method of generating a non-existent *_IN file

1. You will need `EDDFACTOR` and `RVTJ` files from the existing model. Since `EDDFACTOR` is often deleted after the model is completed, you may need to regenerate it by running the existing model for 1 iteration (usually a *Lambda* iteration) For convenience I no-longer delete `EDDFACTOR`.
2. Use the **cpmod** file to copy the required input files to the new model directory. You will also need to copy `EDDFACTOR`, `EDDFACTOR.INFO`, and `RVTJ`.
3. Edit the `batch.sh` file so that the correct atomic data is linked. Create the soft-links by typing **batch.sh ass**.
4. Use `$cmfdist/exe/guess_dc.exe` to generate guesses for departure coefficients of the unknown populations, creating *_IN files in the process. DO NOT DELETE the `EDDFACTOR` file. Alternatively, you could use an existing departure coefficient file from another ionization stage with a similar ionization potential.
5. Edit `MODEL_SPEC`, `VADAT` (and `RVSIG.COL` if necessary) with the desired atomic model changes. In `VADAT` you may need to add the species abundance, and lines of the form

F,F [DIE_XZV]

For CNO species T, T; F,T; and T,F are also viable options — the choice depends on whether resonances have already been included in the photoionization cross-section, and hence should not be doubly counted (in which case the first variable should be F). The second variable should only be true for C III, N III and O V for which states forbidden to autoionize in LS coupling have significant autoionization probabilities. This is true even when the photoionization cross-sections contain resonances, since the photoionization cross-sections have generally been computed in LS coupling. In `VADAT` set `[USE_FIXED_J]` to `TRUE`.

6. Run the model, starting with Λ -iterations. Assuming the correct options are set (as indicated below) in `IN_ITS`, the model will automatically proceed to perform a complete model iteration:
 - (a) Λ -iterations with old radiation field (`[DO_LAM_IT]=T` in `IN_ITS`).
 - (b) Update temperature structure utilizing grey approximation (if `DO_GT_AUTO=T` (default) in `IN_ITS`). For a minor change (e.g., a low ionization species only important in the wind, or an impurity species) this step may not be necessary.

- (c) Λ -iterations with revised radiation field.
- (d) Full iteration with T held fixed (if [FIX_T]=T in VADAT, [DO_LAM_AUTO]=T in IN_ITS)
- (e) Full iteration with variable T (if [FIX_T]=F in VADAT, or if [DO_T_AUTO]=T (default) in IN_ITS).

Older method of generating a non-existent *_IN file

I tend not to use this method – it is simply left as a complicated alternative. If it is a lower ionization stage, simply use the lowest existing ionization stage as the input departure coefficient file. For example, to include Fe III 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 Fe V in a model which has only Fe IV, run WR_F_TO_S with the Fe V oscillator file. For WRDC, use FeIVTX as the input excitation temperature file.

Alternatively, 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 a species with weak influence, it may be best to set [LIN_INT] to .TRUE., so as not to affect the temperature structure.

Copy the XzVOUT files to XzV_IN files, and increase the abundance. Delete (or rename) POINT1, POINT2, SCRTEMP, and EDDFACTOR. 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.

Case 10: Adding X-rays

You wish to add X-rays to an existing model which did not include X-rays. You need to edit the batch.sh file to point to the X-ray emissivity file. You will also need to edit the VADAT file to set [MAX_CF]=1000, and the X-ray parameters: [INC_XRAYS], [FIL_FAC_1], [T_SHOCK_1], [V_SHOCK_1] etc. whose meanings are outlined on page 78. Since adding X-rays can cause huge changes in the populations of high ionization stages (changes of 10^{50} !), I would use the [X_SLOW] option, starting the models with Λ -iterations and [FIXED_T]=T. Once the model is close to reaching the desired filling factors you should check the predicted X-ray flux in OBSFLUX. Since the observed X-ray flux will generally not match that required, you will need to adjust [FIL_FAC_1] and/or [FIL_FAC_2], set [X_SLOW]=F, and restart the model. Note that FIL_FAC_1, and [FIL_FAC_2] in the VADAT file are automatically updated by CMFGEN. The X-ray emission scales as the square of the filling factor.

Computational Checklist for Starting a Model

1. Do I need to delete the POINT* and SCRTEMP files? These must be deleted (or renamed) for a new model, or for a model where you wish to use revised 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 (except if [USE_FIXED_J]=T), 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 in VADAT?
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 in VADAT?
7. If you have changed T_{eff} , is there additional species/ionization stages or processes that should be included in the model?
8. Should I run several Λ -iterations first? Running Λ -iterations with new models is recommended. Similarly, should I start with [FIX_T]=T in VADAT, and [FIX_T_AUTO]=T in IN_ITS?

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.

Troubleshooting

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. You should also 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. The WRDC file will not overwrite existing XzV_IN files. An extension of _IN can be specified by using the hidden option EXT [i.e., WRDC(EXT=_IN)]. As WRDC will not overwrite existing XzV_IN files, they need to be deleted, renamed, or moved. Generally I move the existing XzV_IN files to a subdirectory “jnk”. NB: Be careful not to move/delete GREY_SCL_FAC_IN – this may still be needed when undertaking hydrostatic iterations.

- (c) Increase the number of grid points in the model, especially in the neighborhood of the front. To do this you will need to create a file containing the new R grid (same format as DC files) which can be done by hand or by using \$cmfdist/exe/rev_rdinr.exe. Alternatively you will need to modify the RVSIG_COL file if it is being utilized. An alternative is to 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 does not 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. Possible remedies are:

- (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) Ensure 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., $\dot{M} < 10^{-7} M_{\odot} \text{ yr}^{-1}$).

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 an early iteration, check that input data is correct and consistent (for example, \dot{M} in the VADAT file is the same as that used in RVSIG_COL; GREY_SCL_FAC_IN has not been corrupted).
- (c) If the problem occurs on the last iteration, change the [FRM_OPT] to INT.
- (d) Change [METHOD] option to ZERO, although LOGMON should be stable.
- (e) 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 C IV 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.
- (f) Increase the number of depth points and/or use a finer spatial grid at the outer boundary.

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

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

Possible remedies:

- (a) If it occurs in 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 \dot{M} , used to create the RVSIG_COL file (if used) and in the VADAT file are compatible.
- (c) Check that the GREY_SCL_FAC_IN has not been corrupted. This can occur, for example, when you copy the file from a non converged model, particularly a model having convergence difficulties.

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 is 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 or deleting BAMATPNT. The code will eventually recompute the BA matrix anyway if it continues to detect that the changes are continuing to increase.
 - (d) Average the last 2 iterations, which can be useful if the corrections are oscillating in sign.
6. Poor temperature convergence at a few depths, or T correction goes wild at 1 or 2 depths. This could be a result of [NEW_LINE_BA] being set. For a non-SN model this can be set to false, and you should set [SCL_LN]=T. For a SN model, it may be necessary to set [IND_BA_METH] to a slight higher depth index – the value should be larger than the depths that have convergence issues.
 7. Poor convergence of a single (few) level(s) at a single (few) depth(s).

Possible Remedies:

- (a) Create a file ADJUST_CORRECTIONS to provide a factor to scale all corrections at the specified depths (negative relaxation). In the file you can specify a single depth with the scale factor (e.g., 20, 0.3) or a range of depths (e.g., 20:22, 0.3) with one specification per line. This procedure seems to solve many problems, and can be implemented at any time while the model is running. The scaled corrections are not applied to Λ -iterations.
- (b) Rename the *OUT files to *_IN, making sure that the *OUT files are for the most recent iteration. Alter the bad departure coefficients more reasonable values 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).
- (c) Include more depth points in the neighborhood of the instability.
- (d) Average successive population estimates, since the changes can alter in sign. This can be done using \$cmfdist/exe/do_ng_v2.exe.

8. Asymptotic convergence is poor, with the maximum corrections remaining at the 1% level. Possible Remedies:
- (a) Decrease number of unimportant levels.
 - (b) Use `do_ng_v2.exe` to average the level populations over the last 2 iterations, and restart the model.
 - (c) Pray for guidance.

CMFGEN FILES

Main Model Control Files

IN_ITS

Controls the iteration type and cycle.

[NUM_ITS]	Number of iterations.
[DO_LAMBA_IT]	If TRUE, do lambda-iteration.
[DO_LAM_AUTO]	Automatically switch from Λ -iterations to full iterations (Default=T).
[DO_GT_AUTO]	Do a grey temperature iteration after (automatically) revising USE_FIXED_J (Default=T).
[DO_T_AUTO]	Allow temperature to vary when sufficient convergence has been obtained (Default=F).

The first two keywords must be in the order given above whilst the last three keywords do not need to be present. The first two keywords can 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 to TRUE 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, although as a habit I would include the first 8 options listed below:

[IN_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, but in many cases I start after the first iteration.
[MAX_R]	Used to set maximum radius of model defined as $\text{MAX_R} \times R_c$ where R_c is the connection radius. Note that it is defined in terms of the connection radius (i.e., where the wind joins to the hydrostatic core) – not in terms of the inner radius. If this keyword is NOT set, RMAX/R_* continues to increase (slightly) with each hydrostatic iteration.
[ATOM_DEN]	Density at outer boundary for plane-parallel model. Gives an indication of how far to extend model.
[OB_OPT]	Indicates how depth grid at outer boundary is specified (DEFAULT, SPECIFY, POW, NONE). If SPECIFY (the preferred option), the grid locations are explicitly specified.
[NOB_PARS]	Number of grid locations that are added to the “default” grid to produce a fine grid at the outer boundary. The “default” grid is chosen to satisfy optical depth and velocity constraints.

- [OB_PN] Used to specify the optical depth increments at the outer boundary ($N=1, 2, \dots, \text{NOB_PARS}$). If $\Delta\tau = \tau(2) - \tau(1)$ (before extra point insertion) then the revised τ is $\tau(1 + N) = \tau(1) + \Delta\tau/\text{OB_PN}$. Because a first order boundary condition is used at the outer boundary, the ratio $d\tau(2)/d\tau(1)$ should be large (i.e., Both OB_P1 and OB_P1/OB_P2 [when OB_P2 is specified] should be > 10). O stars with weak winds require the largest value (> 30).
- [RES_REF] Resets reference radius when using old velocity.
- [GAM_LIM] Maximum value for the Eddington ratio (defined using the total opacity). Defaults is 0.98. Only effects models which are VER close to the Eddington limit.
- [VC_ON_SS] Defines the connection velocity (normalized by the sound speed) where the photosphere joins the wind.
- [UP_GREY_SCL] This option updates the GREY_SCL_FAC_IN file. This, in principal, means that the T structure is potentially more accurate after it updates the density structure. This is true, provided the T structure in the hydrostatic region is converged. In practice this option can cause problems when it is not fully converged, since it can cause it be reset to a bad T structure. Default is Fals.
- [TAU_REF] Sets the reference optical depth for g and T_{eff} . The default is $2/3$. This option is useful for W-R models in which the normal photosphere, defined by $\tau = 2/3$ is located in the wind.
- [BETA2] Allows extra freedom with the velocity law around the connection point. Default is BETA (as passed from VADAT), in which case [BETA2] has no effect.

In the wind we have:

$$V(r) = \frac{(V_{\infty} - 2V_c)(1 - R_c/r)^{(\beta + (\beta_2 - \beta)(1 - R_c/r))}}{1 + \exp(R_c - r)/h)}$$

where h is the scale height at the connection point. At the connection point, $\beta_{\text{eff}} = \beta$ while in the wind β approached β_2 .

- [dLOG_TAU] Logarithmic spacing in Tau for new R grid. Default is 0.25.
- [VSCL_FAC] Minimum $V(I+1)/V(I)$ for new R grid (< 1). Recall that $V(I+1) < V(I)$. Default is 0.75D0.

In general, options can be found in \$cmfdist/new_main/do_cmf_hydro_v2.f

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, FULL-LEVELS and IMPORTANT-LEVELS for each ionization stage.
- The maximum number of overlapping lines.

The KEY_WORDS for MODEL_SPEC are explained on page 60.

VADAT

Main file specifying model parameters and options. The various options are explained later in this document (page 62).

Other Control Files

ADJUST_R_DEFAULTS

Control file used with SN models to revise the R grid while the code is running. Used when [REV_RGRID] is set true in VADAT.

[N_ITS]	Number of revisions to be made to R grid.
[STRT_ITS]	First iteration for R grid revision.
[FREQ_ITS]	How often R grid revisions are to be performed.
[GRID_METH]	Space in which R grid is redefined. TAU_SPACE uses a combination of τ and V space to determine the spacing – there is a maximum $\Delta \log V$ and a maximum $\Delta \log \tau$. VEL_SPACE uses constraints on $\Delta \log V$ only.
[GRID_TYPE]	Available options are REFINE, UNIFORM. UNIFORM redefines the entire R grid.
[OB_OPT]	Options are DEFAULT or SPECIFY. SPECIFY indicates that parameters are listed to control grid spacing at the outer boundary.
[NOB_PARAMS]	Number of outer-boundary parameters
[OB_PN]	Parameters for the outer boundary: N=1, ..., NOB_PARAMS. With OB_P1=30, dTAU(2)/dTAU(1) will be 30.
[IB_OPT]	Options are DEFAULT or SPECIFY. SPECIFY indicates that parameters are listed to control grid spacing at the inner boundary.
[NIB_PARAMS]	Number of inner-boundary parameters
[IB_PN]	Parameters for the outer boundary: N=1, ..., NIB_PARAMS. With IB_P1=30, dTAU(ND-2)/dTAU(ND-1) will be 30.

Model Input Files

GAMMAS_IN

Estimate of mean ionization for each atomic species DUM. Generally the GAMMAS file 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 $T/T(\text{grey})$ as a function of Rosseland optical depth. Taken from previously converged model (GREY_SCL_FACOUT). When present it is used to scale $T(\text{grey})$ so as to provide a better estimate of the temperature structure, and hence give significantly better flux conservation, for the first iteration.

RVSIG_COL

Needed when using [VEL_LAW=7] & [VEL_OPT]=RVSIG_COL. Contains R, V, & SIGMA for model in column format. Use an old model file (which can be revised to accommodate a new R_* or \dot{M} using \$cmfdist/exe/rev_rvsig.exe), or create a new version using \$cmfdist/exe/tlusty_vel.exe or \$cmfdist/exe/wind_hyd.exe.

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. Values in this file DO NOT affect the accuracy of a converged model.

XzV_IN

Estimates of departure coefficients as a function of depth for each ionization stage. It is generally the XzVOUT file of a previously converged model, although it can be also created by an option (WRDC) in DISPGEN. Use cpmo to handle their creation from an old model.

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 an integer 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.

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.

T_IN

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

Atomic data files

Generic data files

HYD_L_DATA

Hydrogenic photoionization cross sections for ‘ l ’ states.

GBF_N_DATA

Bound-free gaunt factors for hydrogen.

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 photoionization cross-sections. One file contains data for all species.

RS_XRAY_FLUXES

Fluxes as a function of shock-temperature. Used when including x-rays in the model. Original data was calculated using the old Raymond & Smith code. Newer data has been computed using APEC (Astrophysical Plasma Emission Code) which is a heavily revised version of the Raymond & Smith code. Several data files exist: The file (`$cmfdist/misc/rs_xray_flux_sol.dat`) is the data used with most existing models, but is no longer the preferred data file. Three newer data sets are available: for the galaxy (`gal_xray_hr.dat`), for the LMC (`lmc_xray_fluxes.dat`) and for the SMC (`smc_xray_fluxes.dat`). They were computed by Janos Zsargo using solar, or scaled solar, abundances.

arnaud_rothenflug.dat

List of fits to photoionization cross-sections for elements up to Ni. Used when computing the influence of non-thermal ionizations in supernovae models. Beware: not all ions are presently included in the supplied file.

NUC_DECAY_DATA

Nuclear decay data for supernovae models. File contains isotope masses and half-lives. The file also lists the gamma-rays and their emission probabilities generated by the different decay chains. Beware: some “irrelevant” species can be treated as stable. At present, only 1 and 2-step decay chains are treated.

Species/ion dependent data files

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 NS < NF. Use WR_F_TO_S to assist in creating these files.

DIEXzV

Dielectronic data: Presently taken from Nussbaumer and Storey.

AUTO_XzV_DATA

Contains a list of autoionization level probabilities for levels above the ionization continuum. Only needed for some ions.

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 bookkeeping and archival purposes. It is created/updated on the last iteration.

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 are purely informational. For example, the routine contains an indication of how many (very) weak transitions have been neglected (because of switch settings in VADAT). At the beginning of the model, and on the last iteration, CMFGEN will also output a list of ions that could be deleted, or might be added, to the model. These are a guide only – some ions suggested by CMFGEN may only affect the temperature structure at $\tau = 100$, and hence have no effect on the spectrum. For hot W-R models, it is possible that you may need to include 10 ionization stages of Fe, although in practice (and depending on model purpose) this is usually not necessary for spectral modeling.

OUTGEN also provides a quick means of checking on the progress of a model. The command

grep Maximum OUTGEN

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

grep Lum OUTGEN

will return the radiative luminosity (in the comoving-frame) at the outer and inner boundaries as a function of iteration.

Since the maximum correction is not always representative of the corrections, OUTGEN also lists for each iteration the top 10 fractional corrections which decrease (DEC_VEC) and increase (INC_VEC) variables.

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., POP-CARB, 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. OBS-FLUX also contains information on how the comoving-frame luminosity varies with depth. This provides a check on the accuracy of the flux conservation. For stellar models the luminosity only enters into the transfer solution at the inner boundary (diffusion approximation) – thus the constancy of the luminosity with depth provides a realistic check on the accuracy of the model. The spectrum in this file SHOULD NOT be considered as the final observed spectrum — 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 (observer's frame) in Janskys (assuming $d = 1$ kpc). 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 not 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 – in practice there will be small variations at the 1% level. Extensive testing has shown that errors of 1% have no influence on the results. 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 affected by absorption and by any intrinsic X-ray emission coming from the star and its wind).

Note: The Luminosity output to OBSFLUX is the luminosity in the COMOVING frame. For normal stellar work, this will be very close to the luminosity of the star in the observer's frame. However, for time-dependent SN calculations the CMF luminosity will generally be lower than that computed by integrating over the observed spectrum [since for a static atmosphere $H_{obs} = H_{cmf} + \beta(J_{cmf} + K_{cmf})$]. However, when the luminosity is declining rapidly, the CMF luminosity may actually go above the observer's frame luminosity. This occurs because the CMF explicitly includes time dependence effect and if RMAX is large, you are effectively computing the luminosity at an earlier epoch (there are also additional issues). Fortunately issues related to explicit time dependence are not crucial, and obs_fin should provide the most reliable spectra and luminosities.

Diagnostic output files

BA_ASCII_DN

This file contains the statistical equilibrium equations for a single depth N . N is set/changed by editing `$cmfdist/new_main/subs/generate_full_matrix_v3`. It can be used with `$cmfdist/misc/tst_ba_mat_sol.f` (and a diagonal operator) to check the solution of the rate equations, and to check for near singularities. These files can be deleted at the end of a model run and are irrelevant for most users.

CORRECTION_SUM

This file lists the number of corrections greater than 100%, 10%, 1%, 0.1%, 0.01% and 0.001% as a function of depth. This file is very useful. In most cases, the file will show that each depth has a similar distribution of corrections, and that any differences change 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.

CORRECTION_LINKS

Prints the 5 largest corrections at 5 to 10 depths, and the identification of those corrections with the atomic ionization stage and super-level to which each applies. Originally this had to be done using the `STEQ_VALS` and `MODEL` files. For use when having problems with convergence.

EWDATA

Equivalent widths computed when using CMF or SOB modes. File is empty in BLANKETING mode. Generally empty with CMFGEN calculations, but often used with CMF_FLUX calculations for W-R stars, CSPNs. Data is really only applicable to emission lines (especially with SOB option).

CFDAT_OUT

Continuum frequencies — primarily used by the author for diagnostic purposes.

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 (Hillier 2003). Increasing the number of super levels and/or altering the level assignments should/can reduce the net cooling rate. Generally errors of 20%, or less, 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 larger error at the inner boundary primarily occurs because of limited convergence, and because it is computed using quantities that have already suffered cancellation. 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. The program `$cmfdist/exe/mod_cool.exe` can be used to create a smaller summarized version of GENCOOL (page 109).

HYDRO

Summary of the hydrostatic terms, and radiation force 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. [MASS] in the VADAT file is automatically updated after a hydrostatic iteration has been performed. HYDRO can be rewritten for a new stellar MASS using `$cmfdist/exe/rev_hydro_turb.exe`. This file can be used to check for consistency between the adopted mass-loss rate and velocity law, and the radiation force.

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 (with larger values at some frequencies). 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. If the later occurs, a warning message is output to OUTGEN. In such cases you need to use a smaller step size at the outer boundary. The program `$cmfdist/exe/plt_jc_comp.exe` can be used to plot J and the errors at the outer or inner boundary.

For time-dependent SN model calculations the difference in J(Edd) and J(ray) may be larger. This occurs because J(Edd) depends explicitly on the time while J(ray) only has an implicit dependence (through a dependence on a time-dependent scattering term),

JEW

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

LINEHEAT

Net cooling rates for each bound-bound transition. Defined as $h\nu N_u A_{ul} Z_{ul} / 4\pi$, and it is thus the cooling per steradian. Because of the choice of program units, it is scaled by a factor of 10^{10} . In addition this file contains two running sums of the net cooling rates – the sums differ in how the rates are scaled. I use this file when there are issues with the accuracy of the electron heating/cooling convergence, as indicated in the GENCOOL file, to work out lines that are potentially causing problems. `$cmfdist/exe/plt_ln_heat.exe` can be used to plot data in LINEHEAT. This file is only created on the last iteration, is VERY large, and generally should be deleted after a model is finalized.

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 $d\tau = -f\chi dz$ 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 implemented automatic procedures in CMFGEN to handle these occurrences. They tend to occur more often when the model is unconverged.

NETRATE

Diagnostic file containing the 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. This file is only created on the last iteration, is VERY large, and thus is generally deleted after a model is finalized.

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., $\text{NET_RATE} / \text{TOTAL_RATE} \ll 0.01$ for a converged model). If this condition is not met, there is an ERROR.

STEQ_VALS

On each iteration, 4 arrays are printed out. The first array, of length ND, is simply the radiative equilibrium equation. The second array is the value of each RATE (i.e., statistical equilibrium) equation at each depth. Tabulated as STEQ, with equation depth listed horizontally, and rate equation vertically. 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 equations relate to the ionization equilibrium, species conservation, and if present, ionizations to excited states and Auger ionizations. The third data set lists the merged rate equations in sequential order where degenerate equations have been combined/removed (matrix of size NT \times ND). Also output, under “STEQ SOL”, is the fractional correction to each population — **for historical reasons a –ve correction corresponds to an increase in the variable**. This file can be very useful when diagnosing convergence difficulties. To facilitate interpretation of this file, two additional diagnostic files, CORRECTION_SUM and CORRECTION_LINKS, are created.

While the STEQ_VALS file is not user friendly it is very useful. 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 (corrections are grouped in blocks of 10). Note: If ND > 99 the command is

```
grep 600( 31)# STEQ_VALS
```

(note the space before the 3). 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 \ll than the initial value. NB: The radiative equilibrium equation is set to zero in the STEQ_VALS array when doing a Λ -iteration — this is the reason for the radiative equilibrium equation being printed as a separate vector.

TRANS_INFO

Summary of all bound-bound transitions, in increasing wavelength order. The wavelengths are vacuum for $\lambda < 2000 \text{ \AA}$, and in air for $\lambda > 2000 \text{ \AA}$. Be careful — some files list vacuum for $\lambda > 2000 \text{ \AA}$.

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. Only needed for diagnostic purposes, and can be deleted when a model is finalized.

Scratch Files

These files 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 number) by simply changing the number above IREC and NITSF to 23. POINT1 is also used by the Ng acceleration routines to indicate when the last Ng acceleration occurred. The file is updated after each iteration.

POINT2

Backup copy of POINT1

SCRTEMP

Main scratch file. It saves all atomic populations for each iteration. Thus only results for the current iteration are lost with a code or computer crash. **SCRTEMP is used to restart an existing model** and by the Ng acceleration routine. FREE format, direct access file which may not be portable without modification (although I routinely port it across systems). 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). SCRTEMP can be examined using `$cmfdist/exe/plt_scr.exe`. I tend not to remove the SCRTEMP and POINT files when a model is completed, since these make it easy to run additional iterations in the same directory. However, the commands `$cmfdist/exe/rewrite_scr.exe` and `$cmfdist/com/mvscr.sh` can be used to generate a smaller version of SCRTEMP containing only the last N (default is 2) iterations.

EDDFACTOR

File containing the mean intensity J (RJ in program notation) for each frequency at each depth. Originally the 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, although I routinely transfer the file between LINUX systems, and my Intel MAC..

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 may not be portable.

BAMATPNT

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. CMFGEN uses data stored in this file in when a model is nearly converged – this reduces the model computation time considerably. Remember to delete the file after a model has completed. FREE format and generally 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 (DIAG operator) or 3 files (TRIDIAG operator) 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. They are only output if [WR_PRT_INV] is set to TRUE in VADAT. At the end of an iteration, the files can be deleted using the **dscratch** command (be careful that you don't have other files containing SCRATCH in their name).

Explanation of fields in MODEL_SPEC

MODEL_SPEC is the top level control file for CMFGEN, and defines most of the main variables (see page 11). With VADAT, it controls the nature and the type of model to be run. All parameters need to be included in this file, and every model must include either H or He. For clarity, 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.

[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 although 60 (or higher) is recommended. For O stars, at least 60 points is recommended. When using VEL_OPT=7 (i.e., reading in a TLUSTY core hydrostatic structure) ND must be identical in MODEL_SPEC & RVSIG_COL. For O stars with low mass-loss rates, ND should be larger than 60 since you need at least 5 points per decade of τ in the photosphere, and at least 30 points in the wind.

[NC] Number of rays striking the 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_BOUNDS] Number of bands to be used for 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. Generally set to 70 for smallish models— 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. 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 BLANKETING 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 ($= \text{NXzV_IV} \leq \text{NXzV}$), 20 is the number of super levels ($= \text{NXzV} \leq \text{NXzV_F}$) in the model atom, and 30 is the number of atomic levels ($= \text{NXzV_F}$) 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. For true impurity species, set number of important levels to 0.

[XzV_NSF] It is an obsolete reference used in MODEL_SPEC with an older version of cmfgen. If present in an old model file it should be updated with [XzV_ISF]. [XzV_NSF] 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 ($= \text{NXzV} \leq \text{NXzV_F}$) in the model atom, and 30 is the number of atomic levels ($= \text{NXzV_F}$) in the model atom.

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

[FL_OPT] Optional keyword to automatically change the number of full levels in all species (when absent, NXzV_IF is not changed). This, and the next two keywords were introduced to allow rapid testing of the influence of the model atoms on model results without the need to physically edit NXzV_F etc in MODEL_SPEC, and change the atomic data assignments in batch.sh. Other options could be added to \$cmfdist/subs/fdg_f_to_s_ns_v1.f. When [FL_OPT] is set, NxZV_S is reset to that required by the assigned F_TO_S file – this might be adjusted if the [SL_OPT] is also set.

DO_ALL_LEVS – Sets NXzV_F to use all levels for each ion.

SET_TO_N – Sets NXzV_F to $\text{Min}(N, \text{NXzV_F})$. NB: N should be replaced a numeric value, e.g., 100.

[SL_OPT] Optional keyword to automatically change the number of super levels in all species.

SPLIT_LOW_N – Splits the lower N super levels into individual levels. NB: N should be replaced a numeric value, e.g., 10.

[IL_OPT] Optional keyword to automatically change the number of impurity levels in all species. Must be present when [FL_OPT] or [SL_OPT] is present.

USE_ALL_SL – Sets NXzV_IV to NXzV_S.

SET_TO_N – Sets NXzV_IV to $\text{Min}(N, \text{NXzV_S})$.

UPDATE – Sets NXzV_S to $\text{Min}(\text{NXzV_S}, \text{NXzV_IV} + (\text{NXzV_S} - \text{NXzV_S}(\text{old})))$

NOCHANGE – NXzV_IV remains as the value read in from MODEL_SPEC.

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, while other 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 C III is not included) are ignored.

Additional keywords are continually added to improve the accuracy, convergence properties, and applicability of the code. This will necessitate that 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 subroutine

new_main/mod_subs/rd_control_variables.f.

This routine can be checked for option ordering, and additional info. For logical variables, F can be used instead of FALSE, and T for TRUE. Also please use spaces, rather than a tab, to separate values from their associated keyword.

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., $\tau_{\text{Ross}}=10$ to 100) so that LTE is recovered. Going unnecessarily to very large τ (e.g., $\tau_{\text{Ross}} > 1000$) may cause convergence difficulties. $\tau_{\text{Ross}}(\text{max})$ 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 satisfy the hydrostatic equation. If TRUE, HYDRO_DEFAULTS must be present as a separate file, and [VEL_LAW] must be 7. In this case both [VINP] and [BETA] must also be given in VADAT. When set, R and V are written to SCRTEMP for each iteration. **NB: When set, you must also edit HYDRO_DEFAULTS to specify the number of iterations.**

[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:

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

[VCORE] Velocity in km s^{-1} at R_* when $V_o \gg V_{\text{core}}$. 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 such as V_o (in km s^{-1}).

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

[SCL_HT] Scale height (heff) 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. This 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. This velocity law is an extension of velocity law 3. 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:

$$v(r) = \frac{V_o + (V_\infty - V_{\text{ext}} - V_o)(1 - R_*/r)^{\beta_1} + V_{\text{ext}}(1 - R_*/r)^{\beta_2}}{(1 + V_o/V_{\text{core}} \exp([R_* - r]/h_{\text{eff}}))} \quad (2)$$

[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. For the above, $[\text{VINF1}] = V_\infty - V_{\text{ext}}$ and $[\text{VINF2}] = [\text{VINF1}] + V_{\text{ext}}$

[SCL_HT] Scale height (heff) 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. This is β in the usual β -velocity law. Typical values are in the range 0.5 to 4.

[EPSP1] Needed when $\beta < 1$. Chosen so that $(1 - \epsilon R_*/r)$ is greater than zero at the core, and hence gives a finite dv/dr .

[**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. This is β in the usual β -velocity law. Typical values are in the range 5 to 50.

[**EPFS2**] Needed when $\beta_2 < 1$. Chosen so that $(1 - \epsilon R_*/r)$ is greater than zero at the core, and hence give a finite dv/dr .

[**VEL_LAW**]=7

R, V and SIGMA ($= d\ln V/d\ln r - 1$) 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. For most models, a simple β -velocity law is appended to the hydrostatic structure. A more complicated velocity law can be adopted by setting the key word [BETA2] in HYDRO.DEFAULTS.

[**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 deKoter's format). See newsubs/rd_rv_file_v2.f for further details. A new RVSIG.COL can be created from an old RVSIG.COL file using \$cmfdist/exe/rev_rvsig.exe. Alternatively a new RVSIG.COL file can be created using \$cmfdist/exe/tlusty_vel.exe or \$cmfdist/exe/wind_hyd.exe.

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

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

[**VAR_MDOT**] Logical variable indicating whether the mass-loss rate varies with time, and hence radius. If true, the density structure must be supplied. Used for modeling LBVs, such as AG Car, and for treating winds with a specified density (usually clumped) structure.

[**VM_FILE**] File with density and clumping info for model with variable MDOT. Same format as RV_SIG file except it has two extra columns – the density and the clumping factor. This file could also be used to set R, V, and SIGMA (i.e., utilized as an RVSIG.COL file)

[**VEL_LAW**]=10

Velocity law for SN models. A power law in r (generally a Hubble law) is assumed.

[**VCORE**] Velocity at inner core (km s^{-1}).

[**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.

[VINP] Required terminal velocity, in km s^{-1} , of wind (at infinity).

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

[LSTAR] Total luminosity of star in units of L_{\odot} . This is a fundamental parameter of the model.

[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 $\tau_{\text{Ross}} = 2/3$. For a plane-parallel model, RSTAR is used to define TEFF. **[TEFF] only has an effect when the hydrostatic structure is updated – models in which this is not done will generally have inconsistent luminosities, radii, and [TEFF]. When starting the model do not forget to edit HYDRO_DEFAULTS to indicate the number of hydrostatic iterations to be performed.**

[LOGG] Log of surface gravity (cgs units). Only used when hydrostatic structure is updated. For a spherical star, $\log g$ is specified at $\tau_{\text{Ross}} = 2/3$. For a plane-parallel model, RSTAR is used to define $\log g$.

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

[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 two laws are implemented: EXPO and REXP. No effect if [DO_CL]=FALSE.

EXPO: $f(r) = f_1 + (1 - f_1 - f_3) \exp(-V(r)/f_2) + f_3 \exp(-V(r)/f_4)$

REXP: $f(r) = f_1 + (1 - f_1) \exp(-V(r)/f_2) + (1 - f_1) \exp([V(r) - V_{\text{max}}]/f_3)$

In the above $f_1 = [\text{CL_PAR_1}]$, $f_2 = [\text{CL_PAR_2}]$ etc. For the [EXPO] law, $f_4 = 1$ if $f_3 = 0$.

[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., volume filling factor) at V_{∞} . I 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 $([\text{CL_PAR_1}])^{0.5}$. 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 two 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.

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 was 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 to 100. A much higher value (1000) needs to be adopted when X-rays are included.

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

[AMP_FAC] Amplification factor for large frequency ranges — typically adopt 1.05. Thus
$$\nu_{i+1} = \nu_i \times [\text{AMP_FAC}].$$

[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 0.10. Too large a value will influence the accuracy with which recombination rates are computed.

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

[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 (Typically I 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] – i.e., it should be at least a factor of 2 smaller. 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. Some unsmoothed, or low smoothed, photoionization files are available. Eventually all the photoionization data will be unsmoothed so as to provide greater flexibility. If the data has already been smoothed with a resolution of 3000 km s^{-1} , this option will not have any effect if [SIG_GAU_KMS] is set below 3000 km s^{-1} , since [SIG_GAU_KMS] in CMFGEN is adjusted for the existing smoothing for each ion.
- [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, which is 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 $\text{ABS}(\text{ZNET}-1) < \text{ZNET_VAR_LIM}$. Typically set to 0.01. When $|\text{ZNET}-1|$ 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 as set by ZNET_VAR_LIM.
- [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 logical variable: When true CMFGEN uses a plane-parallel geometry WITHOUT a velocity field. Default is FALSE (i.e., use a spherical model).
- [PP_MOD]** Hidden logical variable: When true, CMFGEN, uses a plane-parallel geometry WITH a velocity field. Default is FALSE (i.e., use a spherical model).
- [INCL_DJDT]** Hidden logical variable: Includes DJDt terms in transfer equation for SN models. For Hubble flow only. Default is FALSE. When running a SN time-sequence, [INCL_DJDT], [USE_DJDT_RTE] and [USE_FRM_REL] should all be TRUE,
- [USE_DJDT_RTE]** Hidden logical variable: Allows the user to force the DJDt transfer routines to be used, even when the DJDt terms are not to be included. Useful for testing, and can also be used for the first model of a time sequence.
- [DJDT_RELAX]** Hidden logical variable: 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 logical variable: Uses MOM_J_REL_VN to solve the momemt transfer equations in the comoving-frame. All relativistic terms may be included. Default is FALSE.
- [USE_FRM_REL]** When true, the fully relativistic ray routine is used to compute the Eddington factors. The default value is TRUE is either [USE_J_REL] or [USE_DJDT_RTE] is true, otherwise it is false.
- [INC_REL]** Hidden logical variable: Includes relativistic terms in the transfer equation when USE_J_REL is TRUE. Default is FALSE.
- [INC_ADV_TRANS]** Includes 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]** Logical variable that tells CMFGEN to use a previously computed J as stored in EDDFACTOR. This can only be TRUE when doing a LAMBDA iteration, and the EDDFACTOR file must exist. It should be set to TRUE when installing new-species, since this allows populations that are consistent with the radiation field to be rapidly computed. USE_FIXED_J is 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, ignores velocity terms when computing continuum.

[JBAR_W_EDD] Computes mean line continuum intensity using Eddington factors. Only used with CMF option (non-blanketed mode).

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

[OB_METH] Option to specify the differencing of the outer boundary condition. Used mainly for development work.

HONJ Default (iterate on H/J)

HALF_MOM Uses half moments to handle the outer boundary condition.

[IB_METH] Optional keyword that supersedes [DIF], but must be consistent with [DIF] if both are present. Primarily for use with SN models.

DIFFUSION Equivalent to DIF=T

ZERO_FLUX Sets the flux to zero at the inner boundary. For the moment solution, this is (almost) equivalent to the diffusion approximation with an inner boundary luminosity of zero. However for the ray-ray solution, we set $I^+ = I^-$ (at the inner boundary) compared with $I^+ = B(T)$. Thus the ZERO_FLUX option will work when the core becomes transparent.

HOLLOW_CORE Assumes the core is hollow and allows for the velocity shift between the near and far sides of the core. This option may be convergence issues since this may cause large changes in some populations close to the inner boundary necessitating a finer grid. This is similar to the ZERO_FLUX option when $V(\text{ND})=0$.

[COH_ES] Switch for coherent electron scattering. For best convergence set key to TRUE. For flux calculations, with CMF_FLUX, set to FALSE. Work on improving the convergence in NON-COHERENT mode is ongoing. To test sensitivity of CMFGEN model to this option, first converge model with [COH_ES]=T. Then run a new model with [COH_ES]=F. Most likely will converge, although issues can occur with the temperature correction. A partial test can be done by setting [FIX_T]=T.

[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 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 en route to a converged model.

Accuracy options

[METHOD] Optical depths in CMFGEN are estimated by the trapezoidal rule with a correction based on the first derivatives using the Euler-McLaurin summation rule. Method determines how the derivatives are estimated. .

ZERO Indicates that the derivatives are zero, and hence the optical depths are to be estimated using a pure trapezoidal rule. Can be a useful option if model is suffering convergence difficulties because of an ionization front.

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

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

$$\left(\frac{d\chi}{dr}\right)_i = \left(\frac{\chi_i}{r_i}\right) \left(\frac{\ln \chi_{i-1} - \ln \chi_{i+1}}{\ln r_{i-1} - \ln r_{i+1}}\right) \quad (3)$$

LOGLIN As for LOGLOG except derivatives estimated using

$$\left(\frac{d\chi}{dr}\right)_i = \chi_i \left(\frac{\ln \chi_{i-1} - \ln \chi_{i+1}}{(r_{i-1} - r_{i+1})}\right) \quad (4)$$

LINLIN As for LOGLOG except derivatives estimated using

$$\left(\frac{d\chi}{dr}\right)_i = \frac{\chi_{i-1} - \chi_{i+1}}{r_{i-1} - r_{i+1}} \quad (5)$$

[VFRAC_FG] Used to facilitate the inclusion of extra points in FG_J_CMF_V11 — the default procedure used to compute the Eddington factors. FG_J_CMF_V11 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 **m** local Doppler widths. 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 **m** local Doppler widths. 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, since 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 CMF mode, this option only applies to the true continuum, where as in blanketing mode, where there is no “distinction” between lines and continua, it applies to all frequencies. In blanketing mode the atmosphere is extended by extrapolation. In other modes a crude approximation is utilized. Preferred default is TRUE — this generally gives a smooth and more realistic run of properties at the outer boundary. Do **NOT** confuse this option with [THK_LINE] — that option is only refers to lines when using the CMF mode.

[REXT_FAC] – Factor to extend outer radius for a thick continuum model. Default is model dependent.

[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 trapezoidal rule. For other moments the appropriate weight (μ, μ^2, μ^3) is specifically taken into account when computing the weight.

[OBC_TYPE] Hidden logical variable: Outer boundary condition type – used by me for development work. Default is 1.

[BC_PAR1] Hidden logical variable: Frequency (10^{15} Hz) below which new boundary condition is adopted – used by me for development work.

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

Line options

[FIX_DOP] Default is TRUE. Indicates the Doppler profiles of fixed width should be used when computing intrinsic line-broadening profiles.

[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 [AMASS_DOP] in a.m.u., and the turbulent velocity [VTURB] in km s^{-1} . One day 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 when [FIX_DOP]=TRUE.

[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. Only used when [FIX_DOP]=TRUE.

[VTURB_MIN] - Minimum turbulent velocity (only used when [FIX_DOP]=FALSE).

[VTURB_MAX] - Maximum turbulent velocity (only used when [FIX_DOP]=FALSE). A linear interpolation in $V(r)$ is used to determine the turbulent velocity at other radii.

[GLOBAL_PROF] Indicates method for determining intrinsic line absorption profiles when [FIX_DOP]=FALSE. Options are:

- NONE** Options for each species determined by [PROF_XzV].
- DOP_FIX** Fixed Doppler width for all species.
- DOP_SPEC** Species dependent Doppler width but depth independent.
- 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.

[OPAC_LIMS] Set prof limits by line to cont. ratio?

[DOP_PROF_LIMIT] Edge limits for Doppler line profile when [OPAC_LIMS]=TRUE. Given as a ratio of line opacity to continuum opacity.

[VOIGT_PROF_LIMIT] Edge limits for Voigt line profile when [OPAC_LIMS]=TRUE. Given as a ratio of line opacity to continuum opacity.

[MAX_ED_PROF] Sets the maximum electron density that will be used in the evaluation of Stark profiles computed via the Griem routine. This is useful, for example, to limit the size of the profile at depth, especially in CMFGEN calculations. NB: Current tabulated stark profiles often have hard wired electron density limits of 10^{17} cm^{-3} . Further, there are issues with He I 4388 above an electron density of 10^{16} cm^{-3} .

[V_PROF_LIM] Sets the the profile limits ($=1/2$ full width) of the intrinsic line profile. Profile is limited to the range set by **[V_PROF_LIM]**, and the integration for rates in integrated over this limit. Does not effect Stark profile, and it is superseded by any limit in file listing line profiles. For CMF_FLUX_V5 the default is 5000 km s^{-1} , while for CMFGEN it is 3000 km s^{-1} . Increasing this limit will often remove (or decrease) errors in OUTGEN or OUT_FLUX regarding profile normalization at high electron densities.

[NORM_PROF] : Indicates that the profile (non-Doppler) area should be normalized to unity. Essential for CMFGEN, and is the default option in both CMFGEN and CMF_FLUX_V5.

[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 (when **FIX_DOP=T**).

[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 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 is generally more stringent than needed, but it does give more accurate profiles with less bleeding to the red (for **OBSFLUX**). Note that **VFRAC_FG** and **VFRAC_MOM** only directly affect the calculation in the comoving-frame. In the observer's frame it only 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** \times **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 . 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 λ smaller than [F.LAM.BEG] or greater than [F.LAM.END]. We use the GLOBAL option for lines with [F.LAM.BEG] $< \lambda <$ [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 logical keyword: Indicates that additional error messages, warnings etc are to be output. Option is not fully implemented. Default is FALSE.

[WRITE.RATES] Default is FALSE. Indicates whether the very large ascii files, NETRATE, TOTRATE, and LINEHEAT should be created.

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 (preferred 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 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 calculated better with CMF_FLUX.

This option has addition features in CMF_FLUX (see §).

[GF.CUT] Omit lines with $gf <$ [GFCUT] and lower level greater than GF.LEV.CUT. At present used only for species with an atomic number $>$ [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 superseded by [MIN.TRANS]. We generally don't want to omit transitions to the ground term, since even weak transitions can be important.

[**AT_CUT**] Allows lines meeting the [**GF_CUT**] criterion to be omitted provided the elemental atomic number is \geq [**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 $0.1 \times \text{ESEC}$ (electron scattering opacity) when, as a consequence of a negative line opacity, it falls below this value. SCRE_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 option for W-R stars, except when there is a problem (see trouble shooting section). For O stars I tend to use SCRE_CHK.

[**He2_RES=0**] Logical variable: Sets the rates in HeII 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.

Options controlling the heating and cooling due to line terms

[**SCL_LN**] Scale the line cooling/heating rates before adding to the radiative equilibrium equation. Set to TRUE for non-supernovae models. 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 fractional 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).

[SCL_SL_OPAC] Alternative option to [SCL_LN] which was developed to handle Type II SN in the inner regions where the optical depth can be very high (e.g., $> 10,000$). In this approach the line opacities and emissivities are both scaled (scaling preserves ratio of η/χ) so that the line cooling from a SL is zero when then the netrate from the same SL is zero. Since the scaling is generally small (e.g. less than a few %) this does not effect the spectrum. Only one of [SCL_SL_OPAC] and [SCL_LN] can be true.

[NEW_LINE_BA] Default is T(rue) for SN, and F(alse) for other models. When true, it switches to an alternative method of evaluating $d(\text{Rad. Eq.})/dT$ which is advantageous at very high optical depths. In the outer region procedure procedure can cause convergence. Thus, for depths 1 to [INDX_BA_METH] we switch to the old method.

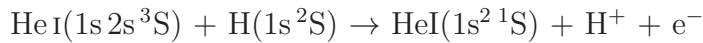
[INDX_BA_METH] . For depths 1 to [INDX_BA_METH]-1 we use the old technique for evaluating $d(\text{Rad. Eq.})/dT$; outside this range we utilize the new technique. The default value for [INDX_BA_METH] is 45. Because of the way we treat strong lines and the cooling, this can effect convergence.

Physical processes 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 W-R models it is generally set to FALSE.

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

[INC_PEN] Include Penning ionization. Penning ionization refers to the following process:



Recall that the $1s\ 2s^3S$ state of HeI is highly metastable.

[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 is 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. This option should only be included when [INC_ADV] is T. This option works for both massive stars and time dependent SN calculations (although different routines are called).

For massive star models this option can generally be set to FALSE. For low-mass loss rate models, adiabatic cooling can be very important for the temperature structure although its effect on the spectrum is generally small (which is why it can generally be neglected). 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.

For SN, adiabatic cooling is related to the material at the previous time step. Thus the treatment is fundamentally different from that used for massive stars.

[INC_ADV] Include advection terms in the rate equations for massive stars with winds. This option is NOT to be used with SN (for SN set [DO_DDT]=T). 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. When advection is important, the ionization state becomes “frozen in”.

[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. Default is 1.0 (i.e., no scaling).

X-ray options

[INC_XRAYS] Include X-rays: Two choices are available: Pure free-free emission (which several underestimates the X-ray emissivity) can be chosen or the X-ray emissivity can be read from a data file which is output from the X-ray code of Raymond and Smith. At present only tables assuming solar, LMC, or SMC abundances available. When X-rays are present, set [MAX_CF]=1000 (i.e., the maximum continuum frequency is 1000×10^{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 emissivity is multiplied by the clumping factor. In this case the X-ray emissivity will be preserved when \dot{M}/\sqrt{f} is held fixed.

[VS_XRAYS] Sets frequency sampling (in km s^{-1}) in the X-ray region. For the SOB/CMF modes, it sets the band over which the X-ray flux is smoothed.

[FIL_FAC_1] Filling factor for first X-ray component (e.g., 1.0×10^{-3}). The X-ray emission is proportional to the square of the (local density) \times (the filling factor). For very low mass-loss rates it may be necessary for the filling factor to approach, even exceed unity, in order to match the observed X-ray luminosities. NB: A second X-ray component can be added with `_2` used to denote the second component.

[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.

NB: 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- Λ 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 1.0×10^{-12} , although the optimal value is model dependent.

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

[XSCL_FAC] When `[XSLOW]=TRUE`, this factor is used to “slowly” increase the X-ray filling factor 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]` (`FIL_FAC_2`) is used.

[V_XRAY] Maximum velocity separation, in km s^{-1} , between evaluations of the X-ray photoionization cross-sections. Default if $0.5 \times \text{VS_XRAYS}$.

Options for beginning a NEW model

[RD_IN_R_GRID] Logical variable which indicates whether a predetermined R grid should be read in. The file should have the same format as the departure coefficient files. Generally set to FALSE – it cannot be used with RVSIG_COL files. The R-grid in RVSIG_COL files can be revised using \$cmfdist/exe/rev_rvsig.exe.

[LIN_INT] Interpolate populations from an “old model.” Should be FALSE when fundamental stellar parameters $[L, R_*, \dot{M}, V(r)]$ have changed. Set the [LIN_INT]=TRUE option when changing the atomic models, computation options, and the number of depth points. NB: If [LIN_INT] =TRUE, no temperature iteration is performed, and the temperature structure is read in.

[POP_SCALE] Scale pops to satisfy abundance equations. Usually TRUE, but setting it to F(alse) might be useful if fudging start populations because model is having convergence difficulties.

[IT_ON_T] When true, CMFGEN iterates on the initial temperature distribution before starting the first iteration. MUST be set to TRUE when initiating new model with NEW stellar parameters. If merely changing the atomic models, or the number of depth points, set to FALSE, and set [LIN_INT] to TRUE. It should also be set to FALSE for SN models in which the ejecta is “optically” thin.

[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 5 when corrections are being read in from GREY_SCL_FAC_IN, otherwise 1 is a more reasonable value. Ideally the value should be larger than [GREY_TAU], since the grey correction provides better accuracy. The temperature computed with this method is subsequently revised using a grey model atmosphere.

[GREY_TAU] Set the temperature to its GREY value for $\tau > [\text{GREY_TAU}]$, 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.

Generally new models start by reading in a table of T/T_{grey} for another similar model from a file called GREY_SCL_FAC_IN (formerly GREY_SCL_FAC). This file should contain ND, and $\tau_{\text{Ross}}, T/T_{\text{grey}}$ in two column format. For current models, a file GREY_SCL_FACOUT is created which contains the relevant data in the appropriate format, and this is copied to GREY_SCL_FAC_IN when the **cpmod** command is used. For very 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).

For SN model, higher values of [T_INIT_TAU] (=20?) and [GREY_TAU] (=10) are often used.

Options specifying method of handling lines.

[TRANS_XzV] Method for treating lines in ionization stage XzV. Available options are BLANK, SOB, and CMF. See description of [GLOBAL_LINE] option discussed above. These specifications need not be present, and are ignored EXCEPT if [GLOBAL_LINE]=NONE.

[DIE_AS_LINE] Treat dielectronic as non-overlapping lines. Preferred option is FALSE, particularly with blanketing calculations. [DIE_AS_LINE]=TRUE 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, are utilized. BE CAREFUL.

Options for assisting convergence

Of these options, [FIX_T] and [FIX_T_AUTO], are the most useful. One useful approach, provided the temperature structure is reasonable, is to set [FIX_T]=T initially. The model can then use Lambda-iterations, and full iterations, to get the populations "consistent" with the radiation field. If [USE_T_AUTO]=T in INITS, [FIX_T] will automatically be adjusted to allow the temperature to vary.

[FIX_ALL_SPEC] When true all species are held fix. This option can be used with [UNFIX_XzV] to allow a single, or multiple ionization stages, to be updated by the CMF-GEN calculation. XzV. Mainly used when adding new species and/or ionization stages. Default is FALSE.

[UNFIX_XzV] Allows a single ionization stage to be removed from the influence of the [FIX_ALL_SPEC] option. Set to 0 to UNFIX the ionization stage

[**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 can be fixed while the other populations are solved for. Usually set to 0, and need not be present in VADAT.

[**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**] When TRUE, impurity species are automatically held fixed. Option is mainly for debugging purposes. If a particular set of levels is causing convergence difficulties, and they have very low populations, they can automatically be held fixed when the other populations are solved for. Usually set to FALSE. A low population level population is currently defined as 10^{-15} of the species population.

[**FIX_T**] Tells CMFGEN to fix the electron temperature. This option was mainly used for debugging purposes but setting it to TRUE initially can help with convergence stability. As rule, I now generally set it to TRUE in VADAT (especially for SN models), and set [DO_AUTO_T]=TRUE in IN_ITS. This will automatically cause CMFGEN to allow the temperature to vary, once the populations have stabilized (in which case CMFGEN will set [FIX_T]=FALSE in VADAT). Setting this option to TRUE is also useful when the temperature is causing convergence difficulties, as often the convergence difficulties are coupled to poor population estimates. [FIX_T] can also be used to compute models where the temperature structure is input, and is not to be changed (but make sure [LIN_INT] is also TRUE).

[**FIX_T_AUTO**] To improve convergence reliability the temperature is typically held fixed until the changes are less than a factor of 5. The temperature is held fixed at all depths with $\tau_{\text{Ross}} < \tau_{\text{Ross}}(\text{Maximum population change on last iteration} < 5)$. [FIX_T_AUTO] is normally set to TRUE, although occasionally it can cause difficulties, and may need to be turned off. Turn it off if you see a discontinuity in temperature at the location where the switch is occurring. Setting to FALSE can speed up some models, but may lead to a more erratic convergence. If you set [FIX_T_AUTO] to FALSE, I strongly recommend beginning a new model with [FIX_T]=TRUE. For SN models I tends to start the model with [FIX_T]=TRUE and [FIX_T_AUTO]=FALSE.

[**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, and lower, optical depths. Normally set to 0. Useful for converging difficult models. `[FIX_T_AUTO]` is an automatic version of this option.

[T_MIN] Approximate minimum value that T can have in a converged model. Usually set to 0.0D0. Can be needed in some models because of exponential overflows when computing LTE populations (i.e., when $T=0.2$ [i.e., 2000 K] 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:
$$\text{OP_SCL_FAC} \times \text{SIGMA(THOMSON)} \times \text{N(ATOM)}.$$

Options for controlling the linearization

[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 has a slower rate of convergence.

[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 (since it can cause very large changes in some populations with unstable oscillations), but switching to this option might accelerate convergence when the temperature needs large adjustments.

[EPS_TERM] Terminate model when maximum fractional change for a FULL linearization is $< [\text{EPS_TERM}]\%$. Typically choose 0.01 to 0.1. Deciding on the level of convergence may be difficult – often the maximum changes is driven by some irrelevant population. One approach, when entering a different model regime, is to decrease EPS_TERM and run a more highly converged model. Then compare the obs_fin file computed with each model. Other checks include seeing how well L is conserved as a function of depth, and checking if the electron cooling balance is satisfied. In practice, numerical errors mean that these comparisons only provide only a check that the model is not grossly in error. Note: Often running a model to a much higher levels of convergence is relatively fast since the linearization matrix is held fixed, and Ng acceleration is generally effective.

[MAX_LIM] Maximum fractional correction to allow for a full linearization iteration. Thus an atomic population can be reduced by a factor of $[\text{MAX_LIM}]$, or increased by a factor of $[\text{MAX_LIM}]$. Typically adopt $[\text{MAX_LIM}]=10$. We use this limit to provide convergence stability - a larger limit might, in some case, provide faster convergence.

[MAX_LAM] Maximum fractional correction to allow for Λ -iteration. Thus an atomic population can be reduced by a factor of $[\text{MAX_LAM}]$, or increased by a factor of $[\text{MAX_LAM}]$. Typically adopt $[\text{MAX_LAM}]=10^5$. 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 $[\text{MAX_CHNG}]$. Typically we adopt 1.0×10^{40} for routine models. A larger value is adopted when introducing a new species whose populations are very uncertain. Although the models stops, the POINT1, POINT2 and SCRTEMP files are updated. You can rewind to the last iteration by editing POINT1. The option is utilized to indicate that the model is likely to have difficulty converging, or that the model may have been incorrectly started/specified.

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

[STORE_BA_INV] Store the inverse of the BA matrix. For very large matrices, this can save computational effort. These are the large scratch files of the form DSCRTATCH01 (etc) discussed earlier.

[N_FIX_BA] When the population corrections are small, the BA matrix is held fixed (see $[\text{BA_CHK_FAC}]$ 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 systems 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] When TRUE, an improved spatial grid is created on which the radiative transfer equation is solved. At present, the linearization on the improved spatial grid is not available with all radiative transfer modes. Useful for improving convergence in the presence of ionization fronts. Convergence is generally inferior to models with [INC_GRID]=F. In CMFGEN it is generally set to FALSE. However, it is utilized in \$cmfdist/exe/cmf_flux_v5.exe to improve the accuracy of spectral calculations (set in CMF_FLUX_PARAM_INIT).

[ALL_FREQ] Use the improved spatial grid for all frequencies. Not used if [INC_GRID] is FALSE, and its recommended value is TRUE.

[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 matrix 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 I adopt 2000, and even 5000 for very large modes. NB: For small models, 200 used to be the recommended value. However for large models, and Λ -iterations, this can significantly increase the required computation time. The file, TIMING, can be checked to see that the update of the BA matrix is not taking too much time (section ADD_PAR).

[**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} for a new model. In practice, the Eddington factors will improve as the model converges. With the completion of a new model the precise value of [ACC_F] will be irrelevant unless you had to compute the EDFACTOR file from scratch and only performed a few iterations.

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. This is especially true when using a diagonal operator. NB: A value larger than ND is set to ND.
- [ITS/NG]** Number of iterations between Ng accelerations. We typically adopt 8.
- [DO_AV]** Perform averaging of oscillating variables in CMFGEN – simple averaging is DONE. Default is FALSE.
- [NOSC_AV]** Only do averaging of population oscillations for [NOSC_AV] iterations. Default is 4. No effect if [DO_AV]=FALSE.
- [ITS/AV]** Number of oscillations between averaging: Default is 8. No effect if [DO_AV]=FALSE.

SN model options

- [**TS_NO**] Sequence number for supernovae model, beginning with model 1. Model 1 must be computed ignoring time derivatives, and hence is usually computed with a fixed temperature structure computed by a hydrodynamical model.
- [**SN_AGE**] Age of SN in days.
- [**DO_DDT**] When true, advection terms, via the comoving derivative, are included in the statistical equilibrium equations. This option is for time-dependent SN models.
- [**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.
- [**SN_T_OPT**] When set to `USE_T_IN`, temperature structure is read in from `T_IN` (same format as `XzV_IN` file). When set to `USE_HYDRO`, it uses the temperature structure in the hydrodynamical model.
- [**JG_W_V**] Include velocity terms when evaluating initial grey temperature structure.
- [**COMP_GREY_LST_IT**] – Indicates whether grey solution should be computed on the last iteration. The computation of the grey solution was an issue for some SN models, but a failure no-longer cause the code to crash.
- [**GAMRAY_TRANS**] When set to `LOCAL`, gamma-rays deposit their energy locally — there is no radiative transport. When set to `ABS_TRANS` a simple approximation (which assumes pure absorption) is used. When set to `NONLOCAL`, data describing the energy deposition is read in from a file.
- [**GAMMA_SLOW**] Add radioactivity decay energy slowly? This option is mainly used for developmental work.
- [**DECNRG_SCLFAC_BEG**] Initial Scale factor for adding decay energy.
- [**N_IB_INS**] Number of points for fine grid at inner boundary (default is 2)
- [**N_OB_INS**] Number of points for fine grid at outer boundary (default is 3)
- [**RMAX_ON_RCORE**] Use when you want to shrink the outer radius of a SN model.
- [**REV_RGRID**] Indicates whether R grid should be automatically revised, after each iteration. Allows better treatment of H ionization fronts.

Additional options for beginning a NEW SN model

- [**PURE_HUB**] Forces flow to be a pure Hubble flow (i.e., homologous expansion) using the age and radius of the SN.
- [**OLD_MFS**] Use old mass scaling when reading SN_HYDRO_DATA.
- [**OLD_MFO**] Use old mass scaling when writing out SN_HYDRO_DATA.
- [**RMAX_ON_RCORE**] Used when want to shrink radius of SN model.
- [**DC_METH**] Set the x-ordinate (i.e. the independent variable) for interpolation of the departure coefficients. Options are , 'ED' (default), 'R', 'LTE' and 'SPH_TAU'.
- [**DC_SPH_TAU**] When true, we interpolate departure coefficients on the spherical TAU scale.
- [**LTE_EST**] Use LTE for the initial estimates.
- [**T_EXC**] This option is used when [LTE_EST]=.TRUE. It sets a minimum excitation temperature when computing level populations. When $T(\text{estimate}) > T_EXC$, LTE populations defined by T are used. When $T(\text{estimate}) < T_EXC$, LTE populations (and hence the ionization structure) are computed using T_EXC. Setting T_EXC to approximately the photospheric temperature (or a little lower) can prevent overflows and other issues when first beginning a SN model for which there is no initial population estimates. In practice, the populations in the outer optically thin regions are more close related to the radiation field (which we characterize by T_EXC) than the local temperature.
- [**STOP_IF_BP**] When true, CMFGEN checks that parameters are consistent. When FALSE only a warning message is given. Mainly used for SN models, and was implemented for testing purposes.

Non-thermal model options

- [**TRT_NON_TE**] When true, CMFGEN computes the non-thermal electron spectrum, and takes into account its influence on the ionization and excitation state of the gas.
- [**NT_NKT**] Number of non-thermal energy bins. Default is 1000.
- [**NT_EMIN**] Minimum energy of non-thermal electrons in eV. Defaults is 1 eV.
- [**NT_EMAX**] Maximum energy of non-thermal electrons in eV. Defaults is 1000 eV.
- [**SCL_NT_CROSEC**] Logical variable to indicate whether excitation cross-sections will be scaled. Scaling factors are read in from NT_CROSEC_SCLFAC. Default is FALSE.
- [**SCL_NT_ION_CROSEC**] Logical variable to indicate whether ionization cross-sections will be scaled. Scaling factors are read in from NT_ION_CROSEC_SCLFAC. Default is FALSE.
- [**NT_IT_CNTRL**] Controls how often we update the non-thermal electron distribution.
- [**NT_OMIT_LEV_SCALE**] Fractional populations below this level are excluded when computing the non-thermal electron spectrum. Default is 1.0×10^{-4} .
- [**NT_OMIT_ION_SCALE**] Excludes ions with population $\text{NT_OMIT_SCALE_FRAC} \times$ (species of ion pop). Default is 1.0×10^{-3} .
- [**NT_SOURCE**] Non-thermal source type - INJECT_DIRAC, CONSTANT or BELL_SHAPE (default).

Auxiliary Programs

All executable names are lower case, and have a .exe extension (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 also 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., H α). 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 $> 10^4$). NB: There is a problem with some of the Lemke Stark profiles for infrared lines.

Running CMF_FLUX

If the model was run in directory r1/, it is recommended that flux calculations be done in the directory r1/obs/, or a sub-directory of similar nomenclature.

Required data files

batobs.sh

Primary control file. It assigns atomic data files, can be used to run multiple spectral calculations with different turbulent velocities, renames output files, and undertakes a continuum only calculation.

CMF_FLUX_PARAMS_INIT

Basic control data. Keywords that have a distinct meaning from those in VADAT are described later in this document. The command file **batobs.sh** copies this file to CMF_FLUX_PARAM which is read by cmf_flux. **batobs.sh** does some simple editing of CMF_FLUX_PARAM to change turbulent velocities, and to perform a continuum calculation. On some operating systems, you may need to make sure CMF_FLUX_PARAM 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/.

FORB_LINE_CONTOL

This simple file is not needed but provides a quick means of omitting forbidden lines (lines between levels of the same parity) when computing the spectrum: File should contain lines with one species (i.e., C2 or CIII) per line, or ALL. For the later case all forbidden lines are deleted.

Atomic data files

As used by CMFGEN. Assigned using

batch.sh ass.

Taken care of by batobs.sh.

Output files from CMFGEN

MODEL, RVTJ, POPDUM (for all species). The **batobs.sh** points to the RVTJ file (usually ../RVTJ to indicate that RVTJ is in directory below the spectral calculation). CMF_FLUX assumes that the other required CMFGEN files are in the same directory as RVTJ.

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 $d = 1$ kpc). It is a raw data file — no smoothing has been done and no effect of rotation is taken into account. The file is initially called OBSFRAME but is renamed by batobs.sh. If spectra with different microturbulent velocities are being computed, the notation obs_fin.10 is used (where 10 is the microturbulent velocity in km s^{-1}). This is done by the batobs.sh file.

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, and can be ignored. The full spectrum OBSFLUX file is copied to obs_cmf by batobs.sh. These files may be deleted. The spectrum in obs_cmf should be very similar to that computed by CMFGEN and obs_fin. obs_cmf will differ from obs_fin because of numerical inaccuracies — photospheric lines will be broadened and wind lines may show a bleeding to the red. Interestingly, EW's tend to be preserved. If obs_fin, obs_cmf, and the CMFGEN OBSFLUX file show broad disagreement (except for resolution issues) there may be a problem. The files can also differ in SN models due to time-dependent effects and/or because a wrong transfer option has been set. For example, using the diffusion approximation may lead erroneously to enhanced fluxes when the core has become optically thin.

A new batobs.sh script allows multiple observed spectra to be computed for different turbulent velocities. The output are termed obs_fin.N, where N refers to the turbulent velocity in km/s. The procedure only computes the CMF spectrum once (ideally for the intermediate turbulent velocity). Similarly, the EDDFACTOR file is reused. Basically, the script sets USE_FIXED_J=T and VTURB before re-running the model.

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. Use an existing model to define this file.

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 OUT_FLUX, 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 may necessitate the CMF_FLUX_PARAM_INIT file 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.

[COH_ES] When FALSE (the preferred option), incoherent scattering due to the thermal motions of the electrons is taken into account. For cmf_flux, this is the preferred option (for CMFGEN preferred option is TRUE).

[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, especially for an O star. Higher values may be necessary when line-photons undergo many scatterings off electrons. On the first 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] \neq DOP_FIX. The turbulent velocity is assumed to have the form

$$\text{VTURB} = [\text{VTURB_MIN}] + ([\text{VTURB_MAX}] - [\text{VTURB_MIN}]) * v(r)/V_\infty$$

[VTURB_MAX] Maximum turbulent velocity in km s^{-1} . Utilized when [GLOBAL_PROF] \neq 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 in the observer's frame. 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].

[GLOBAL_LINE] Switch to indicate which modes are to be used to compute the net-rates (etc) for individual line transitions. Similar to VADAT option but extra flexibility has been added.

BLANK All lines treated in blanketing mode (preferred mode).

BLANK_SPEC All lines treated in blanketing mode, except for lines belonging to ionization stages(s) whose transition type has been specified by [TRANS_XzV]. “_SPEC” may also be added to the [SOB] and [CMF] options.

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 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 calculated better with CMF_FLUX.

[TRANS_XzV] Method for treating lines in ionization stage XzV. Available options are BLANK, SOB, and CMF. See description of [GLOBAL_LINE] option discussed above. These specifications need not be present, and are ignored EXCEPT if [GLOBAL_LINE]=NONE or **_SPEC** has been appended to BLANK, SOB, or CMF. When [GLOBAL_LINE]=NONE, [TRANS_XzV] must be specified for every ionization stage. When **_SPEC** has been appended, [TRANS_XzV] take precedence over the option specified by [GLOBAL_LINE].

[WR_ETA] When true, CMF_FLUX writes η , J_{es} , χ , to direct access files, with the same format as EDDFACTOR. Can be plotted using PLT_JH. Also used by the obsolete OBS_FRAME.

[WR_FLUX] When true, CMF_FLUX writes 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_CMF_FORCE] When true, CMF_FLUX writes 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] When true, CMF_FLUX writes 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 continuum calculation) and [DO_SOB_LINES]=T. Because we use an unblanketed continuum, the force generally exceeds that computed in the CMF. It would probably be more realistic to smooth the blanketed continuum first.

[WR_ION_FORCE] When true, CMF_FLUX writes the radiative line force computed in the CMF for each ion (bound-bound transitions only). The file (ION_LINE_FORCE) is in ascii format, and is self explanatory. Due to non-linear interactions, the contribution by a given ion 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 TRUE.

[WR_IP] When true, CMF_FLUX 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. This file was created to allow comparison of models with interferometric data.

[WR_RTAU] When true, CMF_FLUX writes out $R(\tau_{Ref})$ as a function of impact parameter and frequency. The file is a direct access file and can be plotted using PLT_IP.

[TAU_REF] Reference optical depth for WR_TAU option. Because of the Eddington-Barbier relation, a good choice for [TAU_REF] is 1 (recall the value $2/3$ arise after integrating over all rays [angles]) when you want to plot the characteristic radius of formation along each ray.

[WR_dFR] When true, CMF_FLUX writes out **dFR** as a function of R and frequency. $dFR(I)$ is the flux contribution arising from the spherical volume bracketed by $R(I)$ and $R(I+1)$. Thus $\sum_R dFR$ yields the observed flux (assuming $d = 1$ kpc). The output file is a direct access file and can be plotted using PLT_DFR. This option can be used to determine over what regions a line originates. Unlike the EW and EP options in DISPGEN (which utilize the Sobolev, and other, approximations that only apply to emission lines) this option can be used for both absorption and emission lines.

[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] Option to scale the abundance of an impurity species (NOT H or He). A default value of 1 (i.e., no scaling) is used when the option is not present. This option was 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 should use CMFGEN to compute a new model. Be careful – I would use a distinct names for batobs.sh and CMF_FLUX_PRAM_INIT to avoid scaling abundances accidentally.

DISPGEN

Display package for examining the model atomic populations, plotting, test calculations etc. Routine requires MODEL, RVTJ, POPDUM files, and atomic data files. The code and options are more fully discussed in `$cmfdist/web/dispgen.htm`.

This routine is powerful, and easy to modify. `Dispgen.f` is the main program – options are performed in `$cmfdist/disp/maingen.f`. Using this package it is possible to:

1. Plot T, V, departure coefficients, populations, ionization fractions etc. versus a variety of parameters (e.g., $\log r/R_*$, Ne, column density, depth etc.)
2. Compute approximate equivalents for individual transitions.
3. Compute net-radiative brackets, mean intensities etc.
4. Compare different models.

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 `batch.sh` was the shell script used to run the model under consideration. The internal help does not work – use the supplied web documentation.

DISPGEN will create a lot of files of the form

```
*.sve.
```

These are used so that an option can be repeated. For example,

```
.EW_CIV
```

will use the same parameters last used by the same option (NB: `ew_civ` is the same option as `EQ_CIV`, but the `.sve` filename will be different. Hence, `.EW_CIV` and `.ew_civ` are not equivalent, since they will use parameters from distinct `sve` files). In DISPGEN options must match EXACTLY. The shell command `dsve` will remove ALL files of the form `*.sve`.

In addition,

```
*.box
```

files can be created. These can contain a list of options, with one option per line, that are repeated in sequence (e.g., `.EW_CIV`, `EW_NV`). 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 10^4 K. Most other (y options) then use this as the default X-axis. A few options, because of their nature, use an alternate axis.

DISPGEN operates on only one model at a time, and thus, by itself, cannot compare different models. However, it is fairly trivial to overplot a second model using the WP and RP options in gramon_pgplot. Simply run DISPGEN in alternative window for the second model (I often set the device to /null for this running of DISPGEN). Use this model to create a plot, and send the plot to a scratch, direct access, output file (def is PLT_SCR) using the WP option. This plot is given a name, and can be read in by referring to this name using the RP option. “?” returns the labels, of all known plots. Make sure that the two DISPGEN programs are accessing the **SAME** PLT_SCR file.

PLT_SPEC

Display package for plotting model and observed fluxes. The use of **plt_spec** and its options are more fully discussed in **\$cmfdist/web/plt_spec.htm**. PLT_SPEC contains a single plot buffer – some commands alter the contents of this buffer while other commands move the buffer contents (sometimes with modification) to the buffers associated with the general plotting package (GRAMON_PGLOT).

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 $d=1\text{kpc}$, 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 is also possible to make a crude allowance for interstellar H and H₂, to apply a velocity shift, and to rectify data using a computed continuum. Further, it is possible to smooth the data to match the instrumental resolution, and to modify the observed spectrum for the effects of stellar rotation 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 most used options are RD_MOD, RD_OBS, CNVLV, FLAM, NORM, and ROT which are discussed below.

RD_MOD 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 1 kpc) 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.

CNVLV Allows smoothing of buffer spectrum – either at fixed $d\lambda$ or at a fixed $dV(\text{km s}^{-1})$.

FLAM Sends the data in the buffer to the plot package. At the same time reddening corrections, and a change in the assumed distance, are allowed for. The data in the buffer are not affected. NB: For historical reasons, the FLAM option has nothing to do with the units used for the y-axis – that is set by the YU option.

- NORM** Produces a rectified spectrum by dividing the buffer (containing the model spectrum) by the continuum (as in obs_cont). The data can be sent straight to PGPLOT, or the data buffer can be overwritten.
- ROT** Allows the buffer spectrum to be corrected for the effects of stellar rotation. The adopted default procedure is good for photospheric absorption features, but may fail for wind lines, and photospheric emission lines. The data buffer is overwritten.
- 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 immediately to the plot package, although it can also be read in to the data buffer by setting the keyword OVER to true [i.e., RD_OBS(OVER=T)]. At the top of each file several keywords can be specified. These are used to indicate units, and whether the data is to be scaled.

The keyword **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 “!” in position 1 of a comment line to allow for possible format changes. Possible values for FLUX_UNIT are as follows:

ergs/cm²/s/Ang
 ergs/cm²/s/Hz
 mJy
 Jy
 Jansky
 norm.

On 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 keywords:

- WAVE_UNIT** Angstroms or Micrometers or UM or Hz
AIR_LAM TRUE or FALSE — Used to indicate whether wavelengths > 2000 Å are in air.
SCALE_FACTOR Number — scale factor applied to the flux data.
FLUX_UNIT_n 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 *****. Each data set must also have its own set of keywords which MUST begin with FLUX_UNIT=.

TLUSTY_VEL

Designed to allow CMFGEN 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 [VINFIN] to the largest value in RVSIG.COL. The TLUSTY 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_\odot)
- Rmax** Outer radius of star (in R_*)
- Mdot** Mass-loss rate (in $M_\odot \text{ yr}^{-1}$)
- Vinf** Terminal velocity (in km s^{-1}). Depending on Rmax and β this value may be slightly smaller 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). Low β (< 1) can yield a matching velocity of $< 1 \text{ km s}^{-1}$.
- Beta_h** 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 innermost 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 photosphere 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 yields 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_MULTIMERGE.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.

The basic philosophy is that the plot package should provide reasonable default plots. These defaults can then be modified to make pretty plots. Once the user is happy with a plot, it can be written to a hard file using the Z option. For pretty plots with strings, it is advisable to set an explicit aspect ratio (the default aspect ratio is device dependent). When this is done, plots on the screen will be identical (except for the background color) to those printed.

It is well worth learning how to use this plot package — if nothing else it provides a quick and dirty method of examining CMFGEN output. All of CMFGEN’s (plotting) programs utilize this package. For most purposes you need to know less than half-a-dozen commands.

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 the VEL option before issuing this command.
- LP** Allow a long postscript plot to be created (device CPS only).
- 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 (to make pretty plots)
- 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 - assume the X values are the vertices of the box.
 - H** Histogram- box is drawn from $[x(i-1)+x(i)]/2$ to $[x(i)+x(i+1)]/2$.
 - LG** Plots $\log|Data|$ but indicates by distinct marker data that was originally negative.
- 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

Spectral line measurements and options

- 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 been previously defined, the 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, or from a file which lists previous fits obtained using GF. Two results files, with different formats, are output.

EGF Edit (adjust) the Gaussian fits by hand.

RID Read in a line list that has been created by DISPGEN(LNID). This can be used to label plots. It works best in the optical region where the line density is not too high. The default labeling is for O star spectra in which the continuum is normalized, and where the y-range must cover the interval 1 (or < 1) to 1.2. The [SID] option can be used to the default size/location parameters.

Line and string options

- VC** Define line vectors on the plot using cursor control.
- VF** Read vector definitions from a file.
- VE** Provides an interactive 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** Provides and interactive 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 by 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. One 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 ASCII data file in column format.
- RXY** Read a simple data file that is in ASCII format.
- SXY** Writes ASCII 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 (+, -, / ,*, LG, ALG, R [=const./X]). The default constant allows you to automatically switch between wavelength (angstroms, and assuming vacuum) and units of 10^{15} Hz (or vise-versa).
- YAR** Simple Y axis arithmetic with a constant (+, -, / ,*, LG, ALG, R [=const./Y])
- VAR** Simple arithmetic on two plots (+, -, / ,*). If the X-axes are distinct, the data is interpolated onto a common axis.

History mechanism

- OLF** Open file to log commands.
- CLF** Close log file.
- OIF** Open a previously generated log file for input. Somewhat cumbersome, as a few commands cant be used in this mode (e.g., doing the first hardcopy plot), and previously issued commands can be important. Very useful for generating plots for a sequence of models.
- 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_HYDRO, and if using DO_HYDRO option in CMFGEN. One minor bug is that the code can spend a long time iterating on Ne if Tmin is set too low, and if the corresponding low ionization species are not included. The code can also crash if you have a low Tmin and very high ionization stages. The opacity table is used when adjusting the density and temperature structure to satisfy hydrostatic equilibrium — using the wrong table may affect convergence but does not affect the final solution if convergence is obtained.

To run [main_lte.exe](#) create a sub-directory **lte** in the model directory. In this directory you need to include VADAT and MODEL_SPEC since these indicate which species and ionizations stages will be considered, and the species abundances. These files should be identical to those to be used in the model — it is no longer necessary to edit MODLSPEC. You also need GRID_PARAMS and ltebat.sh. These later files usually do not need to be altered. GRID_PARAMS may need to be altered when switching from O stars to WDs (for example) because the density and temperature range specified in GRID_PARAMS does not cover the desired range. An example GRID_PARAMS file is shown below.

GRID_PARAMS

25	37	!# of T values; # of Electron density values
1.0	15.0	!Tmin, Tmax (10^4 K)
1.0E+06	1.0E+18	!Ne(min), Ne(max)

At the end of the calculation a lot of extraneous files exist. For most purposes, the only useful file is ROSSELAND_LTE_TAB – all other output files can be deleted. The execution of this code is greatly facilitated by using multiple processors.

DO_NG_V2

Reads in SCRTEMP file and does an Ng acceleration. Useful when manually assisting a model to converge. SCRTEMP is automatically updated with the new population estimates, however you must stop and restart the model. Various options are available.

NG Performs an Ng acceleration. Step size, bandwidth, and depths can be specified.

AV Averages the last 2 iterations. This is very useful if some populations are oscillating.

SOR Applies the last set of corrections times SCALE_FAC. The maximum correction is limited to BIG_FAC.

NSR Applies the last set of corrections K times as a geometric series. That is,
$$X_0 = X_1 * (1 + T)^{**K} \text{ where } T = (X_1 - X_2) / X_2.$$

REP Repeats the correction as defined by the last iteration, and a previous iteration (input by the user).

UNDO Replaces a set of depths by the previous iteration.

Recently an automatic plot was added to illustrate the T corrections arising from the NG acceleration, and the T correction arising from the last normal iteration. If the two plots are similar, apart from a simple scaling (you can use the YAR option in PGPLOT to scale the second plot), the NG acceleration is likely to be effective in accelerating the convergence. If the two plots are very different (i.e., they contain significant regimes of different sign) the acceleration should be cancelled (e.g., by \hat{C}). The comparison has been found to be very useful with supernovae models. So far, I have limited experience with non SN models.

For stability reasons, I strongly recommend that you perform a LAMBDA iteration when restarting the model. This can be done by setting both [DO_LAM_IT] and [DO_LAM_AUTO] to TRUE in IN_ITS

Note: You can (Generally) run do_ng.v2 while the model is running – the model only needs to be stopped when you accept the results of the NG acceleration (i.e., POINT1 and SCRTEMP are updated).

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 an entire new species, start with the lowest ionization stage first. This is now the preferred method for adding additional atoms and species. After generating, it is recommended that [USE_FIXED_J] be set to TRUE, and several Λ -iterations be performed. [USE_FIXED_J] should then be set to FALSE, and EDDFACTOR/EDDFACTOR_INFO deleted. This procedure is now handled automatically — CMFGEN will revert to normal iterations once sufficient convergence has been achieved using [USE_FIXED_J] and normal Λ -iterations.

LAND_COL_MERGE & LAND_MULTI_MERGE

Merge several LANDSCAPE pgplots together to make a single postscript file. The plots must have the correct size/aspect ratio if merging is to look correct. Use CPS mode in GRAMON to create the figures. LAND_MULTI_MERGE allows the creation of multiple column plots.

MOD_COOL

Program to rewrite the GENCOOL file into a more convenient format. Two files are written:

GENCOOL_SUM Same format as GENCOOL except that we have summed up over all bound-free rates.

GENCOOL_SORT Similar format to GENCOOL except only the top N rates are printed. The rates are sorted using depths 1, 11, 21 etc. Thus, at depth 20, for example, the rates will not be in order. This file is very useful.

MOD_PRRR

Program to rewrite the XzVPRRR file, for a given species, in a more convenient summary format (output file is XzVPRRR_SUM). Routine also allows the rates, as a function of depth, to be plotted. This allow an easy way to check which processes are directly important for controlling the ionization structure.

N_COL_MERGE & N_MULTI_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.

PLT_CMF_LUM

Plot comoving-frame luminosity and auxiliary vectors from OBSFLUX. Program is designed to check how well the “conserved luminosity” is conserved. Program plots Dr^3/Dt , mechanical term, radioactive energy deposition, and the gas term. Note: For a homologous flow, $Dr^4/Dt = Dr^3/Dt + \text{mechanical term}$.

PLT_IP

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

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 can be read include EDDFACTOR, ES_J_CONV, CHI_DATA, ETA_DATA, FLUX_DATA, CMF_FORCE_DATA, and SOB_FORCE_DATA. Be careful with the Y-axis label, which is not always correct.

PLT_JH_CUR

Plot J and H moments contained in the supernovae data file JH_AT_CURRENT_TIME (or JH_AT_OLD_TIME). Multiple files can be read in, using the RD_MOD option. Options are similar to PLT_JH.

PLT_RJ

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

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. These can, for example, plot both populations and corrections as a function of depth and iteration. Options are listed when you run PLT_SCR.

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.

WIND_HYD

WIND_HYD can be used to generate a RVSIG_COL for use with a new CMFGEN model. Alternatively you can use TLUSTY_VEL, or an existing RVSIG_COL file from a model (especially when generating a model sequence of grid). See README file, and examples, in \$cmdist/lte_hydro. A table of Rosseland mean opacities must be supplied. The density structure is assumed to be hydrostatic below the sonic point, and specified by the velocity law above the sonic point.

WR_F_TO_S

Generates 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).