Modeling the wind and photosphere of massive stars with the radiative transfer code CMFGEN

Jose H Groh
Max-Planck-Institut für Radioastronomie, Auf dem Hügel 69, D-53121 Bonn, Germany
E-mail: jgroh@mpifr.de

Abstract. Massive stars are extremely luminous and characterized by mass loss through radiation-driven stellar winds. The radiation emitted at the stellar surface may interact with the wind, making the analysis of the emerging spectrum a very challenging task. In addition to the luminosity, effective temperature, and surface gravity, several other stellar parameters impact the spectral morphology of these objects, remarkably the mass-loss rate and the wind terminal velocity. That is generally the case for OB supergiants, Luminous Blue Variables, and WR stars. CMFGEN [1] comprises the state-of-the-art in non-LTE radiative transfer and has been successfully applied to the above classes of objects over the last decade. The code assumes spherical symmetry, stationary outflow, and both photospheric and wind lines can be treated in non-LTE. Full line blanketing due to hundreds of thousands of spectral lines is included, as well as wind clumping. Here I discuss the assumptions behind CMFGEN and present examples of models and spectroscopic analyses.

1. Introduction
Massive stars are rare but essential constituents of a stellar population. They are the main contributors to the input of ionizing photons, energy, and momentum into the interstellar medium and playing a key role in the chemical enrichment of their host galaxy. Recent observational studies indicate that stars with initial masses well above 100 $M_\odot$ – and sometimes perhaps as much as 300 $M_\odot$ – are formed in the Milky Way and the Local Group [2]. Theoretical studies based on numerical simulations suggest that stars with high initial masses ($\sim 100 M_\odot$; e.g., [3]) were routinely formed in the early Universe.

Current evolutionary models indicate that very massive stars, with initial masses greater than roughly 40 $M_\odot$, begin their lives as O-type stars burning hydrogen in their cores. After several millions of years, they unavoidably go through an unstable, short-lived stage, known as the Luminous Blue Variable (LBV) phase, when a significant fraction of the stellar mass and angular momentum are lost through winds and giant eruptions. In the current standard picture of stellar evolution, LBVs are progenitors of hydrogen-free Wolf-Rayet (WR) type, helium-core burning stars (see e.g., [4, 5, 6]).

Before going any further, we would like to emphasize the reasons for analyzing spectra of stars in general, as this provides a bridge to compare observations to theoretical evolutionary models. Spectroscopic analysis provides a way to maximize the amount of information extracted from the observations, helping to properly understand massive stars. While photometric observations provide essentially magnitudes and colors, spectroscopy allows one to measure line equivalent widths and ratios, radial velocities, and determined line profiles. However,
to obtain temperatures, luminosities, chemical composition, among other stellar properties, a
careful modeling of the observed spectrum has to be undertaken.

In contrast to low-mass stars like the Sun, massive stars lose mass during their whole lifetime
through radiation-driven stellar winds. This occurs because the radiation field of these stars is
extremely strong, which causes the star to lose mass at enormous rates ($10^{-7}$ to $10^{-3} \text{ M}_\odot\text{yr}^{-1}$).
The stellar wind may become so dense that the stellar photosphere becomes extended and is
formed in a moving layer. Numerous emission lines could then be formed in the wind, veiling
(sometimes completely) the underlying photospheric spectrum. Because the radiation emitted
by the stellar surface interacts with the optically-thick, dense wind, the analysis of the stellar
spectrum is a very challenging task. In addition to the classical stellar qualities such as the
temperature, luminosity, and effective gravity, several other quantities such as the mass-loss
rate and wind terminal velocity may affect the morphology of the spectrum. Complex radiative
transfer models, which include the necessary physics to study the radiation transport across the
atmosphere and wind, are needed to obtain realistic parameters of massive stars.

Here we discuss the state-of-the-art code non-LTE radiative transfer code CMFGEN, its
assumptions, advantages, and limitations, as well as present illustrative examples of models
and spectroscopic analyses. Rather then being an exhausting review on the code itself or
on the extensive science done with CMFGEN, the goal of this paper is to present, from a
user’s standpoint, the essential properties of the code and the basics of spectroscopic analysis
of massive stars using photospheric and wind diagnostics. The reader is referred to [1, 7, 8]
for a comprehensive description of CMFGEN and to [9] for a detailed description of diagnostics
commonly used in the spectroscopic analysis of OB and WR stars.

2. CMFGEN in a nutshell
CMFGEN has been developed and maintained by Dr. D. John Hillier (University of Pittsburgh,
USA), and the code and the associated atomic data are publicly available\(^1\). Analyses with
CMFGEN can potentially provide insights into many subfields of Stellar Astrophysics, and
below we highlight the main applications of CMFGEN (related subfields are in parenthesis):

- derive accurate abundances, stellar and wind parameters (Stellar Evolution);
- derive accurate extreme-UV ($\lambda < 912$ Å) radiation fields (Nebular Photoionization);
- provide fundamental data for the study of starbursts (Star Formation);
- better understanding of the hydrodynamics of winds (Radiation Hydrodynamics);
- testbed of approximate methods that can be used in more complex geometries and in
  inhomogeneous media (Multi-dimensional Radiative Transfer).

Recently, CMFGEN has been adapted to model type II Supernovae, making it possible
to obtain distances and diagnostics of the SN progenitor. The reader is referred to [10] and
references therein for further information about spectroscopic analysis of SNe with CMFGEN,
and hereafter we focus exclusively on massive stars.

2.1. The code suite
CMFGEN comprises not only a single code, and actually a suite of codes are used in the
process of analyzing stellar spectra. While the temperature, atmospheric and wind structures,
and level populations are obtained with CMFGEN itself, the observed spectrum is computed
with a separate code (CMF\_FLUX, see [8]). Many accompanying routines for plotting and
analysis (DISPGEN and PLT\_SPEC) and computation of Rosseland opacities (MAIN\_LTE),
among others, are provided.

\(^1\) http://kookaburra.phyast.pitt.edu/hillier/web/CMFGEN.htm
2.2. The atomic data
As we heard in this Workshop, the quality and self-consistency of atomic data plays a key role in
the spectroscopic analysis and determination of stellar parameters. The atomic data contained
in CMFGEN comes from a variety of sources, which are mainly the Opacity Project \[11, 12\], the
NIST database\(^2\), and from several individuals such as Robert Kurucz\(^3\), Keith Butler (personal
comm.), Sultana Nahar & Anil Prandham\(^4\), and Gary Ferland (personal comm.).
CMFGEN stores atomic data in ASCII files in unique directory structures, with separate files
containing collisional cross sections, oscillator strengths and energy levels, auto ionization rates,
superlevels designation, and photoionization cross sections from the ground and excited states.
As also pointed out by N. Przybilla (in this Volume), one should not assume the atomic data of
a non-standard spectral feature to be correct.
The atomic data format is unique to CMFGEN, and conversion from published data into
CMFGEN is time consuming. Unfortunately, this hampers the portability of atomic data and
test models using atomic datasets from different groups has been done on a very limited basis.

2.3. Transfer options
Depending on the problem to be solved, the user has five options to compute the radiative
transfer in stellar atmospheres with CMFGEN:

- Plane parallel geometry for solving the formal and moment equations;
- Plane parallel co-moving frame for solving the formal and moment equations. Includes the
  zeroth-order terms in \(v/c\) (i.e., we only retain \(v/c\) terms that multiply \(\partial/\partial v\) terms). With
  this option, one can treat monotonic vertical velocity fields in the atmosphere, and the
  radiation transfer is computed in the frame moving with the gas. This has the advantage
  that opacities and emissivities are isotropic.
- Spherical co-moving frame. This option solves the formal and moment equations taking in
  spherical geometry, including the zeroth-order terms in \(v/c\). A radial monotonic velocity
  field has to be specified.
- Spherical co-moving frame relativistic. Similar to option 3, but can treat fully relativistic
  (but stationary) monotonic outflows.
- Spherical time-dependent co-moving frame fully relativistic. Similar to option 4, but
  including time dependence in the moment equation for monotonic outflows. This option is
  still under tests and development as of September 2011.

2.4. Pros and cons of using CMFGEN
CMFGEN includes many physical processes that were neglected in previous codes, allowing the
user to perform a spectroscopic analysis as realistically as possible nowadays. As described
above, CMFGEN can handle spherically-symmetric geometries that is mandatory for modeling
the majority of massive stars (with the exception of B dwarfs, see N. Przybilla, this Volume),
since the presence of a wind makes a plane-parallel approximation invalid. CMFGEN computes
continuum and line formation in the non-LTE regime, and a realistically hydrostatic structure
can be computed until just below the sonic point. This allows the simultaneous treatment of
spectral lines formed in the atmosphere, wind, and in the transition region between the two
regimes, making CMFGEN applicable to the study of massive stars from various evolutionary
states, such as OB, LBV, and WR stars.

\(^2\) http://nist.gov/pml/data/asd.cfm
\(^3\) http://kurucz.harvard.edu
\(^4\) http://www.astronomy.ohio-state.edu/~nahar/nahar_radiativeatomicdata/index.html
Figure 1. Comparison between CMFGEN synthetic spectra appropriate for the O 3.5 star HD 93250 including H and He only (red), H, He, and CNO (blue), and H, He, CNO, Fe, and other Fe group elements (green). The model parameters are: $L_\ast = 1.3 \times 10^6 L_\odot$, $T_{\text{eff}} = 45700$ K, $R_\ast = 18.3 R_\odot$, log $g = 4.0$, $M = 5.6 \times 10^{-7} M_\odot\text{yr}^{-1}$, and $v_\infty = 3000$ km s$^{-1}$. The spectra were smoothed for better visualization. Figure courtesy of D. John Hillier.

As noticed in the early 1990s [13], wind clumping may have a significant impact in obtaining the mass-loss rate of massive stars. CMFGEN allows for the presence of clumping within the wind using a volume-filling factor approach, assuming that material close to the star is unclumped and reaches maximum clumpiness at very large distances. More complex clumping laws can also be taken into account [14].

Line overlap and full line blanketing are also consistently included in CMFGEN through the concept of superlevels, which groups similar energy levels into one single superlevel to be accounted for in the statistical equilibrium equations [15], reducing the computational demand. CMFGEN allows the user to include energy levels and associated transitions from H, He, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Ti, Cr, Mn, Fe, Co, and Ni. Line blanketing plays a major role in the spectroscopic analysis of massive stars, as illustrated in Figure 1. The effects of x-rays are included in an approximate way, as these are crucial in determining the ionization structure of weak winds such as those from O dwarfs [16, 17].

However, it is important that the user is aware of the limitations of CMFGEN. At the moment,
Figure 2. Typical hydrodynamical structure of a CMFGEN model, showing density (left y axis) and velocity (right y axis) as a function of optical depth for a model with $T_{\text{eff}} = 40000$ K, $\log g = 3.50$ and $\dot{M} = 1.4 \times 10^{-5} M_\odot \, \text{yr}^{-1}$. The hydrostatic structure computed with the TLUSTY code (red dashed) or, alternatively, with CMFGEN itself, is connected to a beta-type law (dotted), producing the final CMFGEN hydrodynamical structure (solid line). From [18].

the code does not solve the hydrodynamic equations of the wind, and therefore, a velocity law has to be assumed a priori. In CMFGEN, the velocity law is parameterized by a beta-type law in the wind (or double-beta law), which is joined to the hydrostatic structure just below the sonic point (Fig. 2). Parameters from the velocity law, such as the wind terminal velocity and $\beta$, can be constrained from the observed line profiles though.

In addition, the computational time of a CMFGEN model (typically 10–20 hours) may become a severe limitation, specially in the analysis of large samples of objects. Usually, given the large parameter space to be explored, a grid approach to obtain the best fit model is not feasible, and the user has often to rely on physical insights.

3. Spectroscopic analysis of massive stars with CMFGEN
Here we provide the basic principles behind the comparison between synthetic and observed spectra, and refer the reader to [9] for a more detailed description of some of the diagnostics. In CMFGEN, each model is defined by the effective temperature, luminosity, mass-loss rate, wind volume filling factor, wind terminal velocity, effective gravity (or stellar mass), and by the abundances of the chemical species. This means that, depending on the parameter regime and the amount of data available, one could be able to obtain the above stellar and wind properties by comparison between models and observations.
3.1. Stellar parameters
As opposed to using bolometric corrections, fitting the observed spectral-energy distribution (SED) has become the standard method to constrain the bolometric luminosity of massive stars (assuming the distance is known). The errors associated with this procedure vary between 0.05 and 0.15 dex, depending on the spectral range used for the fit and the quality of the photometry (see e.g., [19, 20, 21, 22, 2, 9]). This technique has the advantage of providing the reddening law towards the target as a byproduct (and thus being less prone to uncertainty in the reddening law), and is particularly well suited for determining the relative changes in the bolometric luminosity in the case of LBVs [20, 21], as shown in Figure 3.

![Figure 3](image)

Figure 3. Comparison between the observed spectral energy distribution of AG Car and CMFGEN models with different bolometric luminosities. The panels are ordered chronologically, and in decreasing effective temperature, from left to right, top to bottom. For each panel we show selected models with $L_\star = 2.2 \times 10^6 \, L_\odot$ (dark green dash-triple dotted line), $L_\star = 1.5 \times 10^6 \, L_\odot$ (black dash-dotted line), $L_\star = 1.1 \times 10^6 \, L_\odot$ (light green solid line), $L_\star = 1.0 \times 10^6 \, L_\odot$ (blue solid line), and $L_\star = 0.7 \times 10^6 \, L_\odot$ (purple dashed line). For a given epoch, models with different $L_\star$ had their $R_\star$ and $\dot{M}$ scaled in order to still fit the observed spectral lines. The gray region corresponds to the uncertainty in the model flux which comes from the luminosity. In all panels, the CMFGEN models were reddened using the Galactic extinction law of [23] with $R_V = 3.5$ and $E(B-V) = 0.65$. Note the trend towards lower luminosity as the effective temperature (radius) decreases (increases) during 2001–2003. The uncertainty in the observed photometry is smaller than the size of the symbols in the UV, optical, and in the near-IR. From [20].
Figure 4. Optical spectra of AG Car taken at 1989 March (black solid line) compared with the best-fit CMFGEN model (red dashed line). The model parameters are: $L_\ast = 1.5 \times 10^6 L_\odot$, $T_{\text{eff}} = 22800$ K, $R_\ast = 58.5 R_\odot$, $M = 70 M_\odot$, $\dot{M} = 1.9 \times 10^{-5} M_\odot\,\text{yr}^{-1}$, $f = 0.10$, and $v_\infty = 300\,\text{km\,s}^{-1}$. From [20].

Once the bolometric luminosity has been obtained, one can use the aid of stellar evolution models to obtain the current and initial stellar masses. Indeed, this method has been applied to suggest that the most massive stars in the Local Group, located at the center of the R136 cluster in the Large Magellanic Cloud, had initial masses between 200–300 $M_\odot$ [2].

The effective temperature is usually obtained from the ionization balance, which can be probed using spectral lines from different ionization stages of the same chemical species. The classical optical diagnostic for O stars is the pair He i $4471$/ He ii $4542$ [9], although lines from Fe iv/v/v1 in the ultraviolet and He i/ He ii in the K-band [9] can also be used. In the case of LBVs, He ii $4542$ is extremely weak and thus He ii $4686$, together with He i $4471$, He i $4713$/5876/6678, are preferred to obtain the He ionization balance [24, 20]. Lines from Si ii/Si iii/Si iv, N i/ N ii, C ii/C iii, and O i/ O ii can also be used as temperature diagnostics in LBVs [20], as well as Fe i/ Fe ii and Mg i/ Mg ii optical lines in cooler LBVs. Figure 4 shows the best fit model of the LBV AG Carinae around $4500\,\text{Å}$, illustrating how both He i and He ii lines can be matched simultaneously for $T_{\text{eff}}=22\,800$ K.

In OB stars, the effective gravity can be constrained from the pressure-broadened wings of Hydrogen lines. The Balmer H\(\delta\) and H\(\gamma\) lines are the classical diagnostics, since the influence of the stellar wind on these lines is minimized. However, in massive stars with dense winds, such as LBVs and WRs, even H\(\delta\), H\(\gamma\), or the Paschen lines have emission components caused by the wind. Notice in Figure 4, in the case of AG Car, how H\(\gamma\) shows a P-Cygni profile and thus cannot be used for constraining log\,g. Usually, log\,g (and thus masses) of WRs and LBVs cannot be obtained from spectroscopic analysis, with the exception of cool LBVs with thin winds, such as W243 in the massive cluster Westerlund 1 [25].

3.2. Wind parameters

The presence of a stellar wind affects significantly the spectral morphology. Constraints on the mass-loss rate are usually obtained from non-saturated lines with high optical depth. While UV resonance lines of N v, C iv, Si iv, N iv can be employed in the case of massive stars with
relative weak winds, recombination lines such as Hα (or another strong H line) or He II 4686 are the classical $M$ diagnostics for stars with dense winds such as LBVs and WRs. Figure 5 illustrates the effects of $M$ on the morphology of Hα in the case of an O dwarf, showing that this line turns from an absorption to emission profile as $M$ increases [17].

Since there is overwhelming evidence for massive star winds being clumped (at least) on small scales (see contributions in [26]), recombination lines actually constrain the ratio $Mf^{-0.5}$, where $f$ is the wind volume filling factor. Diagnostics that are not dependent on the density squared, such as the electron scattering wings [13] or non-saturated UV resonance lines (e.g., O V 1371 in O stars, [27]), can be used to constrain $f$ (Figure 6).

The wind terminal velocity is best constrained using metallic resonance lines, which are usually found in the UV. In O stars and WRs, the classical diagnostics are N V 1240, Si IV 1393–1403, C IV 1548–50, and N IV 1718 [9], while in LBVs, these are C II 1334–1335, C III 1175, and Mg II 2800–2802 [20]. Whenever UV spectroscopic is unavailable, for instance for stars with large amounts of reddening, a lower limit to $v_\infty$ can be obtained either using the width of the emission or the velocity of the maximum absorption of H and He lines in the optical and near-IR.

4. CMFGEN and Gaia
As described above, an accurate spectroscopic analysis of massive stars usually relies on multi-wavelength diagnostics, or at least makes use of a large fraction of the UV, optical, or near-IR bands. Since Gaia will cover a relatively narrow spectral region in medium spectral

![Figure 5. Variations in the Hα morphology as a function of the adopted $\dot{M}$. All synthetic spectra were computed with CMFGEN, and the one with the strongest emission has log($\dot{M}/M_\odot$yr$^{-1}$) = −6.00, while the one with strongest absorption has log($\dot{M}/M_\odot$yr$^{-1}$) = −9.22. Models with intermediate values of $\dot{M}$ are shown alternatively with solid and dashed lines for clarity. From [17].]
resolution around 8500 Å, an unambiguous determination of stellar and wind parameters of individual targets will likely not be possible. However, the broad spectral range of the Gaia spectrophotometric mode (3300–11500 Å) will provide spectral energy distributions that could be used to roughly constrain the evolutionary stage of individual targets by determining whether these are OB-type, LBV, or WR stars. In this context, follow-up ground-based surveys, such as the Gaia-ESO public survey (see Blomme, this Volume), will play a key role in maximizing the amount of massive star science that will be obtained out of the Gaia survey.

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