On line contribution functions and examining spectral line formation in 3D model stellar atmospheres

A. M. Amarsi\textsuperscript{1}\textsuperscript{*}

\textsuperscript{1}Mount Stromlo Observatory, Australian National University, Weston Creek, ACT 2611, Australia

Accepted 2015 June 22. Received 2015 June 13; in original form 2015 February 16

ABSTRACT

Line contribution functions are useful diagnostics for studying spectral line formation in stellar atmospheres. I derive an expression for the contribution function to the absolute flux depression that emerges from three-dimensional ‘box-in-a-star’ model stellar atmospheres. I illustrate the result by comparing the local thermodynamic equilibrium (LTE) spectral line formation of the high-excitation permitted OI 777 nm lines with the non-LTE case.

Key words: line: formation – radiative transfer – methods: numerical – stars: atmospheres

1 INTRODUCTION

The fundamental parameters of stars such as their effective temperature, surface gravity, and chemical composition are not observable quantities: rather, they must be inferred using model stellar atmospheres (Bergemann 2014). Three-dimensional (3D) hydrodynamic ‘box-in-a-star’ models (Nordlund 1982) are increasingly being used in this context (Ludwig et al. 2009; Magic et al. 2013a; Trampedach et al. 2013). These present a huge improvement over classical 1D hydrostatic models on account of their ab initio treatment of convective energy transport in the outer envelope that can realistically reproduce the shifting, broadening and strengthening of spectral lines by convective velocity fields and atmospheric inhomogeneities (Nordlund 1980; Asplund et al. 1999). Inferred logarithmic abundances can suffer errors as large as ±1.0 dex when modelled in 1D (Collet et al. 2008).

Visualizing and understanding spectral line formation in three dimensions is non-trivial. Contribution functions (de Jager 1952; Gurtovenko et al. 1974) are useful tools to that end. They can be interpreted as probability density functions for line formation in the atmosphere (Staude 1972; Magain 1986) and are often used to infer the mean formation depths of spectral lines. The line intensity contribution function (Magain 1986) represents the contribution from different locations of the atmosphere to the depression in the normalized intensity. This quantity is commonly used to study lines in a solar context (Caffau et al. 2008). Since stars are in general not resolved, often more relevant is the line flux contribution function, (Albrow & Cottrell 1996), which is instead formulated in terms of the depression in the absolute flux.

Since all parts of the stellar atmosphere contribute to its observed flux profile, the line flux contribution function is a function of 3D space. Albrow & Cottrell (1996) derive it in the context of 1D model stellar atmospheres, i.e. assuming plane-parallel symmetry. To apply it directly to a 3D model would be to treat the atmosphere as an ensemble of 1D columns i.e. it would be a 1.5D approximation (Kiselman & Nordlund 1995). This is undesirable because the effects of horizontal radiative transfer are entirely neglected. Another approach is to compute the plane-parallel contribution function on a horizontally-averaged, \(<3D>\) model. This approach is still not ideal, because it neglects the effects of the atmospheric inhomogeneities which characterize real stellar atmospheres.

In this paper I present in §2 a derivation for the line flux contribution function that is valid in three dimensions. To illustrate the result, I explore in §3 the formation of the high excitation permitted OI 777 nm lines in a 3D hydrodynamic stagger model atmosphere (Magic et al. 2013a). I present a short summary in §4.

2 THE 3D LINE FLUX CONTRIBUTION FUNCTION

2.1 Concept

The flux depression at frequency ν from a star of radius R measured by a distant observer is proportional to the total emergent intensity depression,

\[
A_\nu \propto \frac{1}{\pi R^2} \int \int (I_\nu - I_\nu) \, \rho \, d\rho \, d\phi ,
\]

in the cylindrical polar coordinate system depicted in Figure 1: the polar axis intersects disc-centre and is directed...
towards the observer, $I_ν$ is the specific intensity and $I'_ν$ is the specific continuum intensity, at some position on the disc, in the direction of the observer. The line flux contribution function $C_ν$ must satisfy

$$A_ν = \int_0^{2\pi} C_ν (r) \, r \, dr \, dz \, dΩ. \tag{2}$$

Crucially, the integration is not performed over vertical height as in the plane-parallel derivation of Albrow & Cotrell (1996), but over the entire 3D volume in which the line may form. This is the entire volume of the 3D model atmosphere; $r$ thus specifies a position in this box.

In what follows, equation (1) is manipulated into the form of equation (2), and thereby $C_ν$ is inferred. The contribution function $C$ to the integrated line strength $A = \int A_ν \, dν$ is also found, and satisfies $C = \int C_ν \, dν$.

2.2 Derivation

Along any given ray, $I_ν$ and $I'_ν$ satisfy the respective transport equations,

$$\frac{dI_ν}{dz} = \alpha_ν (S_ν - I_ν), \tag{3}$$

$$\frac{dI'_ν}{dz} = \alpha'_ν (S'_ν - I'_ν), \tag{4}$$

where $z$ is the path distance, increasing upward towards the observer. The linear extinction coefficient $\alpha_ν$ and the source function $S_ν$ are, in terms of their line and continuum components,

$$\alpha_ν = \alpha^l_ν + \alpha^c_ν, \tag{5}$$

$$S_ν = \frac{S^l_ν + \alpha^c_ν S^c_ν}{\alpha_ν} \tag{6}$$

(Hubeny & Mihalas 2014).

Following Magain (1986), an effective transport equation for the intensity depression $D_ν \equiv I'_ν - I_ν$ is found by subtracting equation (3) from equation (4),

$$\frac{dD_ν}{dz} = \alpha_ν (S'^{\text{eff}}_ν - D_ν), \tag{7}$$

where the effective source function is

$$S'^{\text{eff}}_ν = \frac{\alpha^l_ν}{\alpha_ν} (I'_ν - S'_ν). \tag{8}$$

In terms of the optical depth along the ray $dτ_ν = -dα_ν \, dz$, equation (7) is expressed as

$$\frac{dD_ν}{dτ_ν} = D_ν - S'^{\text{eff}}_ν. \tag{9}$$

The formal solution is found by integrating from $τ_ν = 0$ to $τ_ν \to \infty$,

$$D_ν = \int S'^{\text{eff}}_ν e^{-τ_ν} \, dτ_ν. \tag{10}$$

Neglecting proportionality factors, the flux depression is obtained by substituting equation (10) into equation (1),

$$A_ν = \int_0^{2\pi} \int_0^\pi \int_0^\infty α_ν S'^{\text{eff}}_ν e^{-τ_ν} \, dz \, dρ \, dφ, \tag{11}$$

where the integrand is evaluated with the constraint that the emergent rays are directed towards the observer. As the observer is very far from the star, the emergent rays are parallel to each other. Consequently, the last equation is written in terms of an infinitesimal volume element,

$$A_ν = \int_\text{star} α_ν S'^{\text{eff}}_ν e^{-τ_ν} \, d^3r. \tag{12}$$

The integration in equation (12) is performed over the entire volume of the star. 3D box-in-a-star models of stellar atmospheres have Cartesian geometry and span a minute surface area of the stars they represent (Freytag et al. 2012; Magic et al. 2013a). The flux spectrum from the modelled star is (approximately) reproduced by shifting the box tangentially across the spherical surface. This is represented by two integrations: one over the volume of the box and the other over the unit hemisphere. Again neglecting proportionality factors,

$$A_ν \approx \int_0^{2\pi} \int_0^\pi \int_0^\infty α_ν (r; Ω) S'^{\text{eff}}_ν (r; Ω) e^{-τ_ν(r; Ω)} \, d^3r \, dΩ \, dν, \tag{13}$$

where the functional dependence of the integrand has been made explicit for clarity. The position vector $r$ specifies a position within the box, and the solid angle $Ω$ specifies the direction of the emergent rays. The infinitesimal solid angle satisfies $dΩ = dm \, dφ$, where $m = \cos θ$. After changing the order of integration, the contribution function is inferred to be,

$$C_ν (r) = \int_0^{2\pi} \int_0^\pi α_ν (r; Ω) S'^{\text{eff}}_ν (r; Ω) e^{-τ_ν(r; Ω)} \, dΩ \, dν. \tag{14}$$

This represents the contribution of a point within the box to the observed absolute flux depression in the line, at frequency $ν$. The integrated line strength contribution function follows immediately,

$$C (r) = \int_0^{2\pi} \int_0^\pi α_ν (r; Ω) S'^{\text{eff}}_ν (r; Ω) e^{-τ_ν(r; Ω)} \, dΩ \, dν. \tag{15}$$

2.3 Rotational broadening

Line broadening caused by the rigid rotation of the star must be included during post-processing. This broadening


will affect the monochromatic quantity $A_\nu$ and hence $C_\nu$. Following Dravins & Nordlund (1990), the broadened specific intensity is,
\[
I^\text{broad}_\nu = B [I_\nu] ,
\]
where $B$ is a functional which broadens its argument according to,
\[
B [x (v, \theta, \phi)] = \frac{1}{2\pi} \int x (v - V \sin \iota \sin \theta \cos \psi, \theta, \phi) \, dv .
\]
Here $v = c \frac{\nu}{c \cos \iota}$ is the Doppler speed, $V$ is the rotation speed of the star in the line forming region, $\iota$ is the inclination angle of the rotation axis with respect to the observer, and the integral is over an interval of $2\pi$. Retracing the steps above, one obtains a rotationally-broadened contribution function,
\[
C_\nu (r) = \int B [\alpha_\nu (r; \Omega) S^{\text{eff}}_\nu (r; \Omega) e^{-\tau_\nu (r; \Omega)}] \, d\Omega .
\]
(In this expression, it is necessary to move $B$ within the integral of equation (10). This is valid because the atmosphere is assumed to be sufficiently shallow that $V$ does not vary across its depth.)

This integrated line strength $A_\nu$ should not be affected by the rotation of the star (Gray 1992). The adopted broadening formalism is consistent with this: integrating equation (17) across the line profile,
\[
\int B [x (v, \theta, \phi)] \, dv = \int x (v, \theta, \phi) \, dv ,
\]
which implies that the contribution function $C$ is not affected by the rotation of the star.

### 2.4 Mean formation depth

The interpretation of the contribution function as a probability density function for line formation (Staude 1972; Magain 1986) suggests a formalism for defining the mean formation value of some quantity $\delta$ with respect to a line,
\[
E [q] = \frac{\int q (r) C (r) \, d^3r}{\int C (r) \, d^3r} ,
\]
and the variance might then be defined in the usual way as $E [q^2] - E [q]^2$. For example, $E [q = \log_{10} \tau_{500}]$ may be used to define the mean formation value, where $\log_{10} \tau_{500}$ is the logarithmic radial optical depth at wavelength $\lambda = 500$ nm, a standard measure of depth in stellar atmospheres.

### 2.5 Relationship to the line flux response function

A related spectral line formation diagnostic is the response function: the linear response of the line to a perturbation in the atmosphere (Meyn 1971; Beckers & Milkey 1975; Caccin et al. 1977). The line flux response function $R_\nu$ must satisfy
\[
\delta A_\nu = \int R_\nu (r) \delta \beta (r) \, d^3r ,
\]
where $\beta$ is an atmospheric parameter (such as temperature).

Following Magain (1986), the response function is obtained by adapting the above derivation. The effective transport equation equation (7) is perturbed so that $D_\nu \rightarrow D_\nu + \delta \beta D_\nu^\text{b}$, and the equation for $D_\nu$ is solved,
\[
\frac{dD_\nu^\text{b}}{dz} = \alpha_\nu \left( S^{\text{eff},1}_\nu - D_\nu^\text{b} \right) ,
\]
where the perturbed effective source function is,
\[
S^{\text{eff},1}_\nu = \frac{\partial S^{\text{eff}}_\nu}{\partial \beta} + \frac{1}{\alpha_\nu} \frac{\partial \alpha_\nu}{\partial \beta} \left( S^{\text{eff}}_\nu - D_\nu \right) .
\]
The response function is then found by following the previous derivation, but with $D_\nu$ and $S^{\text{eff}}_\nu$ replaced by $D_\nu^\text{b}$ and $S^{\text{eff},1}_\nu$, respectively,
\[
R_\nu (r) = \int \alpha_\nu (r; \Omega) S^{\text{eff},1}_\nu (r; \Omega) e^{-\tau_\nu (r; \Omega)} \, d\Omega .
\]
and the response function to the integrated line strength is $R = \int R_\nu \, d\nu$.

Response functions can be used to study the sensitivity of a spectral line to specific atmospheric variables (Achmad et al. 1991). To identify the line forming regions, however, contribution functions must be used.

### 2.6 Comparison to the plane-parallel line flux contribution function

In the limit of plane-parallel symmetry, the integrand in equation (14) loses its dependence on the azimuthal angle $\phi$: $\alpha_\nu (r; \Omega) \rightarrow \alpha_\nu (z; \mu)$, $S^{\text{eff}}_\nu (r; \Omega) \rightarrow \tau_\nu (z; \mu)$, $\tau_\nu (r; \Omega) \rightarrow \tau_\nu (z; \mu)$, $\mu$ is the geometrical height and $\tau_\nu$ is the radial optical depth. The 3D contribution function $C_\nu$ thus tends to a plane-parallel contribution function $C_\nu^{pp}$,
\[
C_\nu^{pp} (z) = 2\pi \int \alpha_\nu (z; \mu) S^{\text{eff}}_\nu (z; \mu) e^{-\tau_\nu (z; \mu)/\mu} \, d\mu .
\]
This expression is the same as that derived by Albrow & Cottrell (1996) in the context of 1D models, i.e. with the implicit assumption of plane-parallel symmetry.

### 3 Example: 3D Non-LTE Spectral Line Formation

The high excitation permitted OI 777 nm lines are known to show departures from local thermodynamic equilibrium (LTE) (LTE: Sedlmayr 1974; Kiselman & Nordlund 1995; Fabbian et al. 2009). A temperature snapshot of a 3D hydrodynamic model atmosphere taken from the STAGGER-grid (Collet et al. 2011; Magic et al. 2013a) was used. The model was of a typical turn-off star, with effective temperature $T_{\text{eff}} \approx 6430$ K, logarithmic surface gravity (in CGS units) $\log_{10} g = 4$, and solar-value

\[1\] After expressing the contribution function in that paper with respect to geometrical height instead of radial optical depth, they are the same to a factor of $2\pi$, which arises from those authors integrating over spherical polar angle $\mu$ instead of solid angle $\Omega$.
Figure 2. Material temperature in a vertical slice of a temporal snapshot of a 3D hydrodynamic stagger model atmosphere (Magic et al. 2013a). The snapshot has effective temperature \( T_{\text{eff}} \approx 6430 \text{K} \), logarithmic surface gravity (in CGS units) \( \log_{10} g = 4 \), and solar-value abundances. Contours of standard logarithmic optical depth \( \log_{10} \tau_{\nu,0} = -3, -1, 1 \) (from top to bottom) are overdrawn.

The LTE and non-LTE contribution functions in this snapshot slice are shown in Figure 3. They are both normalized such that the maximum value of the non-LTE contribution function is 1.0. The contribution functions reveal how to derive the contribution function to the absolute flux depression that emerges from 3D box-in-a-star model stellar atmospheres. The result can be used like other 1D contribution functions (Magain 1986; Alibow & Cottrell 1996) to help one visualize and understand spectral line formation in stellar atmospheres.

The LTE and non-LTE contribution functions in this snapshot slice are shown in Figure 3. They are both normalized such that the maximum value of the non-LTE contribution function is 1.0. The contribution functions reveal how to derive the contribution function to the absolute flux depression that emerges from 3D box-in-a-star model stellar atmospheres. The result can be used like other 1D contribution functions (Magain 1986; Alibow & Cottrell 1996) to help one visualize and understand spectral line formation in stellar atmospheres.

4 SUMMARY

Flux profiles observed from stars have contributions from all parts of its atmosphere: thus, the line flux contribution function is a function of 3D space. In this paper I have shown how to derive the contribution function to the absolute flux depression that emerges from 3D box-in-a-star model stellar atmospheres. The result can be used like other 1D contribution functions (Magain 1986; Alibow & Cottrell 1996) to help one visualize and understand spectral line formation in stellar atmospheres.

ACKNOWLEDGEMENTS

I thank Martin Asplund and Remo Collet for advice on the original manuscript, and Jorrit Leenaarts for providing MULTI3D. This research was undertaken with the assistance of resources from the National Computational Infrastructure (NCI), which is supported by the Australian Government.

References

Achmad L., de Jager C., Nieuwenhuijzen H., 1991, A&A, 250, 445
Alibow M. D., Cottrell P. L., 1996, MNRAS, 278, 337
Asplund M., 2005, ARA&A, 43, 481
Asplund M., Grevesse N., Sauval A. J., Scott P., 2009, ARA&A, 47, 481
Asplund M., Nordlund Å., Trampedach R., Stein R. F., 1999, A&A, 346, L17
Beckers J. M., Milkey R. W., 1975, Sol. Phys., 43, 289
Bergemann M., 2014, Analysis of Stellar Spectra with 3-D and NLTE Models. Springer International Publishing, pp 187–205
Caccin B., Gomez M. T., Marmolino C., Severino G., 1977, A&A, 54, 227
Caffau E., Ludwig H.-G., Steffen M., Ayres T. R., Bonifacio P., Cayrel R., Freytag B., Plez B., 2008, A&A, 488, 1031
Carlsson B. G., 1963, Methods in Computational Physics, 1, 1
Carlsson M., Judge P. G., 1993, ApJ, 402, 344
Collet R., Asplund M., Trampedach R., 2008, Mem. Societa Astronomica Ital., 79, 649
Collet R., Magic Z., Asplund M., 2011, Journal of Physics Conference Series, 328, 012003
de Jager C., 1952, The hydrogen spectrum of the sun. Druk: Excelsior Foto-Offset, s-Gravenhage
Dravins D., Nordlund A., 1990, A&A, 228, 203
Fabbian D., Asplund M., Barklem P. S., Carlsson M., Kiselman D., 2009, A&A, 500, 1221
Freytag B., Steffen M., Ludwig H.-G., Wedemeyer-Böhm S., Schaffenberger W., Steiner O., 2012, Journal of Computational Physics, 231, 919
Gray D. F., 1992, The observation and analysis of stellar photospheres.. Cambridge Univ. Press, Cambridge
Gurtovenko E., Ratnikova V., de Jager C., 1974, Sol. Phys., 37, 43
Beckers J. M., Milkey R. W., 1975, Sol. Phys., 43, 289
Bergemann M., 2014, Analysis of Stellar Spectra with 3-D and NLTE Models. Springer International Publishing, pp 187–205
Caccin B., Gomez M. T., Marmolino C., Severino G., 1977, A&A, 54, 227
Caffau E., Ludwig H.-G., Steffen M., Ayres T. R., Bonifacio P., Cayrel R., Freytag B., Plez B., 2008, A&A, 488, 1031
Carlsson B. G., 1963, Methods in Computational Physics, 1, 1
Carlsson M., Judge P. G., 1993, ApJ, 402, 344
Collet R., Asplund M., Trampedach R., 2008, Mem. Societa Astronomica Ital., 79, 649
Collet R., Magic Z., Asplund M., 2011, Journal of Physics Conference Series, 328, 012003
de Jager C., 1952, The hydrogen spectrum of the sun. Druk: Excelsior Foto-Offset, s-Gravenhage
Dravins D., Nordlund A., 1990, A&A, 228, 203
Fabbian D., Asplund M., Barklem P. S., Carlsson M., Kiselman D., 2009, A&A, 500, 1221
Freytag B., Steffen M., Ludwig H.-G., Wedemeyer-Böhm S., Schaffenberger W., Steiner O., 2012, Journal of Computational Physics, 231, 919
Gray D. F., 1992, The observation and analysis of stellar photospheres.. Cambridge Univ. Press, Cambridge
Gurtovenko E., Ratnikova V., de Jager C., 1974, Sol. Phys., 37, 43

Figure 3. The contribution function $C_{z}$ across the oxygen triplet (777.25nm to 777.85nm in vacuum) corresponding to the snapshot slice in Fig. 2, in LTE (left) and in non-LTE (right). These quantities are expressed in the same arbitrary units. Contours of standard logarithmic optical depth $\log_{10} \tau_{500} = -3, -1, 1$ (from top to bottom) are overdrawn.

Hubeny I., Mihalas D., 2014, Theory of Stellar Atmospheres. Princeton Univ. Press, Princeton, NJ
Kiselman D., 1993, A&A, 275, 269
Kiselman D., Nordlund A., 1995, A&A, 302, 578
Leenaarts J., Carlsson M., 2009, in Lites B., Cheung M., Magara T., Mariska J., Reeves K., eds, The Second Hinode Science Meeting: Beyond Discovery-Toward Understanding Vol. 415 of Astronomical Society of the Pacific Conference Series, MULTI3D: A Domain-Decomposed 3D Radiative Transfer Code. p. 87
Ludwig H.-G., Caffau E., Steffen M., Freytag B., Bonifacio P., Kucinskas A., 2009, Mem. Societa Astronomica Ital., 80, 711
Magain P., 1986, A&A, 163, 135
Magic Z., Collet R., Asplund M., Trampedach R., Hayek W., Chiavassa A., Stein R. F., Nordlund Å., 2013a, A&A, 557, A26
Magic Z., Collet R., Hayek W., Asplund M., 2013b, A&A, 560, A8
Mein P., 1971, Sol. Phys., 20, 3
Nordlund A., 1980, in Gray D. F., Linsky J. L., eds, IAU Colloq. 51: Stellar Turbulence Vol. 114 of Lecture Notes in Physics, Berlin Springer Verlag, Numerical simulation of granular convection - Effects on photospheric spectral line profiles. pp 213–224
Nordlund A., 1982, A&A, 107, 1
Sedlmayr E., 1974, A&A, 31, 23
Staude J., 1972, Sol. Phys., 24, 255
Trampedach R., Asplund M., Collet R., Nordlund A., Stein R. F., 2013, ApJ, 769, 18