Temperature Correction Methods

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Abstract. In this paper we discuss numerical methods and algorithms for the solution of NLTE stellar atmosphere problems involving expanding atmospheres, e.g., found in novae, supernovae and stellar winds. We show how a scheme of nested iterations can be used to reduce the high dimension of the problem to a number of problems with smaller dimensions. As an example of these sub-problems, we discuss our temperature correction procedure as applied to expanding atmospheres and to irradiated atmospheres such as those found in extrasolar giant planets.

1. Introduction

Our group has developed the very general non-LTE (NLTE) stellar atmosphere computer code PHOENIX (Hauschildt 1992; Hauschildt 1993; Hauschildt et al. 1995; Allard & Hauschildt 1995; Hauschildt et al. 1996; Baron et al. 1996; Hauschildt, Baron, & Allard 1997; Baron & Hauschildt 1998; Hauschildt & Baron 1999) which can handle extremely large model atoms as well as line blanketing by hundreds of millions of atomic and molecular lines. This code is designed to be both portable and flexible: it is used to compute model atmospheres and synthetic spectra for, e.g., novae, supernovae, M, L, and T dwarfs, irradiated atmospheres of extrasolar giant planets, O to M giants, white dwarfs and accretion disks in Active Galactic Nuclei (AGN). The radiative transfer
in PHOENIX is solved in spherical geometry and includes the effects of special relativity (including advection and aberration) in the modeling.

The PHOENIX code allows us to include a large number of NLTE and LTE background spectral lines and solves the radiative transfer equation for each of them \textit{without} using simple approximations like the Sobolev approximation. Therefore, the profiles of spectral lines must be resolved in the co-moving (Lagrangian) frame. This requires many wavelength points (we typically use 150,000 to 300,000 points). Since the CPU time scales linearly with the number of wavelength points, the CPU time requirements of such calculations are large. In addition, (NLTE) radiative rates for both line and continuum transitions must be calculated and stored at every spatial grid point for each transition, which requires large amounts of storage and can cause significant performance degradation if the corresponding routines are not optimally coded.

An important problem in stellar atmosphere calculations is to find a consistent solution of the very diverse equations that describe the various physical processes. We have developed a scheme of nested iterations that enables us to separate many of the variables (e.g., separating the temperature correction procedure from the calculation of the NLTE occupation numbers). This allows us to compute far more detailed stellar atmosphere models than was previously possible (see references for details).

In order to take advantage of the enormous computing power and vast aggregate memory sizes of modern parallel supercomputers, both potentially allowing much faster model construction as well as more sophisticated models, we have developed a parallel version of PHOENIX (Baron et al., this volume).

In this contribution we concentrate on the description of our temperature correction procedure as it applies to both expanding atmospheres and to the irradiated atmospheres of extrasolar giant planets (Barman, Hauschildt, & Allard 2001).

2. Temperature Correction Procedures

2.1. The Unsöld-Lucy Method

Given the iterative nature of the model atmosphere problem, it is necessary to apply a correction to the source function at the end of each iteration so that the radiative equilibrium constraint is satisfied. One powerful and simple technique for determining the correction is the Unsöld-Lucy (U-L) procedure. The following derivation for spherically symmetric irradiated atmospheres closely follows that of Lucy (1964) which was intended for plane parallel LTE atmospheres with the traditional "isolated" upper boundary condition.

The derivation begins with the time independent, static, spherically symmetric transfer equation,

\[ \mu \frac{\partial I}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial}{\partial \mu} I_{\nu} = (\kappa_{\nu} + \sigma_{\nu}) \rho (S_{\nu} - I_{\nu}), \]

with the symbols having their usual meanings.
The moments of the transfer equation are obtained by applying the operators \( \frac{1}{2} \int_{-1}^{1} d\mu \) and \( \frac{1}{2} \int_{-1}^{1} \mu d\mu \) to equation 1. These moments are:

\[
-(\kappa_\nu + \sigma_\nu)\rho H_\nu = \frac{\partial}{\partial r}(K_\nu) + \frac{(3K_\nu - J_\nu)}{r} \quad \text{and} \quad (2)
\]

\[
\frac{\partial}{\partial r}(r^2 H_\nu) = -(\kappa_\nu + \sigma_\nu)\rho r^2 (J_\nu - S_\nu), \tag{3}
\]

where \( H_\nu \) is the Eddington flux \( (H_\nu = \frac{1}{2} \int_{-1}^{1} I_\nu \mu d\mu) \) and \( K_\nu \) is the second moment of the radiation field \( (K_\nu = \frac{1}{2} \int_{-1}^{1} I_\nu \mu^2 d\mu) \).

Integrating over frequency and inserting the mean opacities,

- \( \kappa_P = \frac{1}{B} \int_{0}^{\infty} \kappa_\nu B_\nu d\nu \) (Planck mean)
- \( \kappa_J = \frac{1}{J} \int_{0}^{\infty} \kappa_\nu J_\nu d\nu \) (absorption mean)
- \( \kappa_H = \frac{1}{H} \int_{0}^{\infty} (\kappa_\nu + \sigma_\nu) H_\nu d\nu \) (flux mean)

equations 2 and 3 become \(^1\)

\[
-\rho\kappa_H H = \frac{\partial}{\partial r}(K) + \frac{(3K - J)}{r} \quad \text{and}
\]

\[
\frac{\partial}{\partial r}(r^2 H) = -\rho\kappa_P r^2 (\frac{\kappa_J}{\kappa_P} J - B). \tag{4}
\]

Note that the approximate expression for the source function, \( S_\nu = (\kappa_\nu B_\nu + \sigma_\nu J_\nu)/(\kappa_\nu + \sigma_\nu) \), has been assumed.

The first equation in 4 may be transformed into a first order linear equation by introducing the variable Eddington factor, \( f = \frac{K}{J} \). The equations in 4 are straightforward to solve by introducing an integrating factor, \( q \). Expressed in the following way,

\[
\ln(r^2 q) = \int_{r_c}^{r} \frac{(3f - 1)}{r'f} dr' + \ln(r_c^2), \tag{5}
\]

\( q \) is often called the sphericity factor which was first introduced by Auer (1971). After applying the integration factor, the equations in 4 become

\(^1\)Note that the subscript \( \nu \) has been dropped to indicate wavelength integrated quantities.
\[
\frac{\partial}{\partial \tau} (q f \mathcal{J}) = q \frac{\kappa_H}{\kappa_P} \mathcal{H} \quad \text{and} \quad \frac{\partial}{\partial \tau} (\mathcal{H}) = \left( \frac{\kappa_J}{\kappa_P} \mathcal{J} - B \right),
\]

where \( \mathcal{J} = r^2 J \), \( \mathcal{H} = r^2 H \), \( B = r^2 B \), and \( \partial \tau = -\rho \kappa_P \partial r \). The moment equations have now been reduced to functions of only one independent variable, the Planck mean optical depth \( \tau \).

Let \( \Delta B(\tau) \) be the correction to the source function such that, upon the next iteration, the correct target flux, \( H_{\text{target}} \), is obtained at each layer. The moment equations then become

\[
\frac{\partial}{\partial \tau} (q f' \mathcal{J}') = q \frac{\kappa_H}{\kappa_P} \mathcal{H}_{\text{target}} \quad \text{and} \quad \frac{\partial}{\partial \tau} (\mathcal{H}_{\text{target}}) = \left( \frac{\kappa_J}{\kappa_P} \mathcal{J}' - B - \Delta B \right),
\]

where \( f' \) denotes quantities to be determined at the end of the next iteration.

One of the benefits of introducing the means defined above is that their ratios do not change much from one iteration to the next. Therefore, one may assume that \( \frac{\kappa_H}{\kappa_P} = \frac{\kappa_H}{\kappa_P} \) and \( \frac{\kappa_J}{\kappa_P} = \frac{\kappa_J}{\kappa_P} \). Using these approximations and further assuming \( f = f' \), we may subtract the equations in 7 from those in 6 obtaining two equations with just two unknowns:

\[
\frac{\partial}{\partial \tau} (q f \Delta \mathcal{J}) = q \frac{\kappa_H}{\kappa_P} \Delta \mathcal{H} \quad \text{and} \quad \frac{\partial}{\partial \tau} (\Delta \mathcal{H}) = \left( \frac{\kappa_J}{\kappa_P} \Delta \mathcal{J} + \Delta B \right),
\]

where \( \Delta \mathcal{J} = \mathcal{J} - \mathcal{J}' \) and \( \Delta \mathcal{H} = \mathcal{H} - \mathcal{H}_{\text{target}} \). By explicitly assuming \( f = f' \), we are also assuming that \( f = \frac{\Delta \mathcal{H}}{\Delta \mathcal{J}} \), a fact that will become important later.

Solving the first equation in 8 for \( \Delta \mathcal{J} \) gives

\[
\Delta \mathcal{J}(\tau) = \frac{1}{q(\tau)f(\tau)} \left( q(0)f(0)\Delta \mathcal{J}(0) + \int_0^\tau q(\tau') \frac{\kappa_H(\tau')}{\kappa_P(\tau')} \Delta \mathcal{H}(\tau')d\tau' \right).
\]

Inserting \( \Delta \mathcal{J} \) into the second equation in 8 and solving for \( \Delta B \) yields an expression for the correction to the source function:
\[ \Delta B(\tau) = \frac{d\Delta H}{d\tau} + \]

\[ \frac{\kappa_J}{\kappa_P} \left( q(0)f(0)\Delta J(0) + \int_0^\tau q(\tau')\frac{\kappa_H(\tau')}{\kappa_P(\tau')} \Delta H(\tau')d\tau' \right) \frac{1}{q(\tau)f(\tau)}. \]

Instead of computing the gradient of the flux, it is simpler to use the fact that

\[ \frac{d\Delta H}{d\tau} = \frac{dH}{d\tau} = \frac{\kappa_J}{\kappa_P} J - B. \]

Using the second Eddington approximation, \( \Delta H(0) = J(0) \), and inserting equation 11 into equation 10, the correction to the source function becomes,

\[ \Delta B(\tau) = \frac{\kappa_J}{\kappa_P} J(\tau) - B(\tau) + \]

\[ \frac{\kappa_J}{\kappa_P} \left( 2q(0)f(0)\Delta H(0) + \int_0^\tau q(\tau')\frac{\kappa_H(\tau')}{\kappa_P(\tau')} \Delta H(\tau')d\tau' \right) \frac{1}{q(\tau)f(\tau)}. \]

All quantities on the right hand side of equation 12 are available upon completion of each iteration and, so, the correction to the source function may be determined. In practice, however, applying a correction to the gas temperature is more convenient than applying a correction to the source function directly. Using the Stefan-Boltzmann law and differentiating \( \dot{B} \) with respect to \( T \) gives the temperature correction at each layer;

\[ \Delta T(\tau) = \frac{\Delta B(\tau)}{4\sigma T(\tau)^3 r^2}. \]

The expression, \( \frac{\kappa_J}{\kappa_P} J - B \), is always small at large optical depth where the gas pressures and densities are high and \( S \rightarrow B \). Therefore, the first term on the right hand side of 12 only generates a correction in the optically thin parts of the atmosphere. The second term is most important in the optically thick regions and also ties the thermal structure to the prescribed target flux.

2.2. The Condition of Radiative Equilibrium in Expanding Atmospheres

The time-independent radiation energy equation is obtained by integrating the special relativistic spherically symmetric radiation transport equation (SSRTE) over \( \mu \) and \( \nu \) and can be written as (Mihalas & Weibel-Mihalas 1984)

\[ e \frac{\partial I}{\partial \tau} + \frac{\partial}{\partial \mu} (fI) + g \frac{\partial}{\partial \lambda} (\lambda I) + hI = \eta - \chi I \]
with

\[ e(r, \mu) = \gamma(\mu + \beta) \]
\[ f(r, \mu) = \gamma(1 - \mu^2) \left[ \frac{1 + \beta \mu}{r} - \gamma^2(\mu + \beta) \frac{\partial \beta}{\partial r} \right] \]
\[ g(r, \mu) = \gamma \left[ \frac{\beta(1 - \mu^2)}{r} + \gamma^2 \mu(\mu + \beta) \frac{\partial \beta}{\partial r} \right] \]
\[ h(r, \mu) = \gamma \left[ \frac{\beta(1 - \mu^2)}{r} + \gamma^2(1 + \mu^2 + 2\beta \mu) \frac{\partial \beta}{\partial r} \right] \]

where \( J = 1/2 \int_0^\infty \int_{-1}^1 I_\lambda d\mu d\lambda \) is the wavelength integrated mean intensity and \( H = 1/2 \int_0^\infty \int_{-1}^1 \mu I_\lambda d\mu d\lambda \), and \( K = 1/2 \int_0^\infty \int_{-1}^1 \mu^2 I_\lambda d\mu d\lambda \) are the wavelength integrated first and second moments of the specific intensity.

This equation is closely coupled to the hydrodynamic equations of the moving matter and, therefore, is best solved using a radiation-hydrodynamic method. However, in astrophysical applications the density structure of an expanding model atmosphere is often given by a previous hydrodynamic simulation. In this case, it is a reasonable approximation to assume radiative equilibrium in the Lagrangian frame, i.e., to assume that each element of material absorbs the same amount of radiative energy that it emits. The condition of radiative equilibrium equation in the Lagrangian frame is then simply given by

\[ \int_0^\infty (\eta_\lambda - \chi_\lambda J_\lambda) \ d\lambda = 0 . \]

The equivalent condition for the wavelength integrated Eddington flux, \( H \), can be written in the form (Mihalas & Weibel-Mihalas 1984)

\[ \frac{\partial (r^2 H)}{\partial r} + \beta \frac{\partial (r^2 J)}{\partial r} + \frac{\beta}{r} r^2 (J - K) \]
\[ + \gamma^2 \frac{\partial \beta}{\partial r} r^2 (J + K + 2\beta H) = 0 \] (14)

where \( H = 1/2 \int_0^\infty \int_{-1}^1 \mu I_\lambda d\mu d\lambda \), and \( K = 1/2 \int_0^\infty \int_{-1}^1 \mu^2 I_\lambda d\mu d\lambda \) are the first and second moments of the specific intensity.

The accuracy of the assumption of radiative equilibrium in the Lagrangian frame can be checked only by performing a detailed radiation-hydrodynamic modeling of actual problems. It is not clear, beforehand, how much radiative energy is converted into kinetic energy or internal energy and vice versa. However, the temperature correction method we describe in this paper can also be applied to problems where the net amount of radiative energy, \( E_{\text{rad}} \), emitted or absorbed by the moving material does not vanish but is a known quantity, \( E_{\text{ext}} \), (for example, mechanical or convective energy flux). In this more general case Eq. (14) is replaced by

\[ \frac{\partial (r^2 H)}{\partial r} + \beta \frac{\partial (r^2 J)}{\partial r} + \frac{\beta}{r} r^2 (J - K) \]
\[ + \gamma^2 \frac{\partial \beta}{\partial r} r^2 (J + K + 2\beta H) = E_{\text{ext}} \] (15)
The value of the Eddington flux, as measured by an external observer, \( H_{\text{obs}} \), is a given model parameter. Using the transformation formulae between the Lagrangian and the Eulerian systems for the wavelength integrated moments of the radiation field (e.g., Mihalas & Weibel-Mihalas 1984),

\[
J_{\text{obs}} = \gamma^2 \left( J + 2\beta H + \beta^2 K \right),
\]
\[
H_{\text{obs}} = \gamma^2 \left\{ (1 - \beta^2)H + \beta(J + K) \right\},
\]
\[
K_{\text{obs}} = \gamma^2 \left( K + 2\beta H + \beta^2 J \right)
\]

we can compute the Euler system radiation field moments (denoted by the subscript “obs”) from the corresponding quantities in the Lagrangian frame which are assumed to be known from a previous solution of the SSRTE. We note that the above transformation is crucial if \( \beta \geq H/J \) (dynamic diffusion, see Mihalas & Weibel-Mihalas 1984), this situation arises in supernovae but is not important in novae or stellar winds.

If we assume that the geometry factors, \( f_{\text{obs}} \equiv J_{\text{obs}}/H_{\text{obs}} \), and \( g_{\text{obs}} \equiv K_{\text{obs}}/H_{\text{obs}} \), are not sensitive to the temperature, we can compute an improved estimate for the Eddington flux in the Lagrangian frame \( H^{(1)} \) at \( \tau = 0 \) by means of the expression

\[
H^{(1)} = \gamma^2 \left\{ \left( 1 + \beta^2 \right) H_0 - \beta H_0 \left( f_{\text{obs}} + g_{\text{obs}} \right) \right\},
\]

where \( H_0 = \) is the target luminosity in the observer’s frame (an input parameter).

Using \( H^{(1)} \) as an initial condition and assuming that the Lagrangian frame geometry factors \( f \equiv J/H \) and \( g \equiv K/H \) are only weakly dependent on the temperature, we can solve Eq. (15) as an ordinary differential equation by means of standard numerical methods. This procedure gives the improved run of \( H^{(1)}(\tau) \) in the Lagrangian frame.

### 2.3. Temperature Correction Procedure in Expanding Atmospheres

In the outermost level of the nested iteration scheme we also iterate for the temperature structure of the atmosphere using a generalization of the Unsöld-Lucy temperature correction scheme to spherical geometry and NLTE model calculations. This has proven to work very well even in extreme NLTE cases such as nova and supernova atmospheres. The temperature correction procedure requires virtually no memory and CPU time overheads. The Unsöld-Lucy correction scheme uses the global constraint equation of energy conservation to find corrections to the temperature that will fulfill energy conservation better than the previous temperatures. We have found it to be more stable than a Newton-Raphson linearization scheme and it allows us to separate the temperature corrections from the statistical equations, dramatically improving the numerical stability of the overall iteration procedure. Note that the Unsöld-Lucy procedure will work only if the radiation field at every wavelength is consistent with the absorptive and scattering opacities (i.e., that the scattering contribution to \( J \)'s are correctly accounted for), otherwise the computed mean opacities
and integrated \( J, H, \) and \( K \) would be locally inconsistent and the temperature correction scheme will simply not work.

The first term in Eq. (12) corresponds simply to a \( \Lambda \) iteration term and will thus provide too small temperature corrections in the \textit{inner} parts of the atmosphere (but work fine in the outer, optically thin parts). The second term of Eq. (12), however, is the dominant term in the inner parts of the atmosphere. It provides a very good approximation to the temperature corrections \( \Delta T \) deep inside the atmosphere. Following Unsöld (1968), we found that it is sometimes better to modify this general scheme by, e.g., excluding the contributions of extremely strong lines to the opacity averages used in the \( \Delta T \) calculations because they tend to dominate the average opacity but do not contribute as much to the total error in the energy conservation constraint.

\textit{Irradiated Atmospheres} \hspace{1em} In the presence of irradiation, the atmosphere’s upper boundary is altered to account for the incident flux. Requiring strict energy conservation implies that all of the energy received by the secondary must be re-radiated into space either as a contribution to the thermal flux or as reflected light. As a result, the target flux \((H_{\text{target}})\) is now given by:

\[
H_{\text{target}} = H_{\text{ext}}(\tau) + \sigma T_{\text{int}}^4
\]

where \( H_{\text{ext}}^{\text{ext}}(\tau) \) is the extrinsic Eddington flux \((H_{\nu}^{\text{ext}} = \frac{1}{4\pi} P_{\nu}^{\text{inc}})\) that has penetrated down to optical depth \( \tau \) and \( \sigma T_{\text{int}}^4 \) is the total flux due solely to the secondary’s intrinsic energy source.

The U-L temperature correction procedure derived above is formally correct even in the case of strong irradiation (so long as the correct target flux is supplied). However, for the reason described below, the correction scheme can become unstable when \( H_{\text{ext}}(\tau) \gg \sigma T_{\text{int}}^4 \). With a few modifications, stability can be achieved (Barman 2002).

The first modification concerns the Eddington approximation used to relate \( \Delta J \) with \( \Delta K \). If the total intensities are separated into intrinsic and extrinsic components then, similarly, the moments of the radiation field may also be separated into intrinsic and extrinsic components; \( J = J_{\text{ext}} + J_{\text{int}}, K = K_{\text{ext}} + K_{\text{int}} \) and \( H = H_{\text{ext}} + H_{\text{int}} \). Since the radiation from the primary is constant, the extrinsic components will also be constant from one iteration to the next apart from changes that will occur in the opacities (due to changes in \( T \)). Therefore, \( \Delta J \) becomes \( \Delta J = J_{\text{int}} - J'_{\text{int}} \) and likewise for \( \Delta K \) and \( \Delta H \). Thus, in the case of irradiation, equation 8 should involve only intrinsic mean intensities \((J_{\text{int}})\). Also, since we used \( f \) to relate \( \Delta J \) with \( \Delta K \), \( f \) must also involve only intrinsic quantities. Therefore \( f \), in equation 12, should be replaced by \( f_{\text{int}} = \left( \frac{\Delta J}{\Delta K} \right)_{\text{int}} \) and assume that \( f_{\text{int}} = f'_{\text{int}} \).

The second modification is slightly more subtle and involves \( \kappa_H \) (defined above). The second correction term in equation 12 applies a “torque” on the temperature structure in a direction governed solely by the sign of \( \Delta H \); if \( \Delta H(\tau) = H(\tau) - H_{\text{target}}(\tau) < 0 \), then the temperature is too cool and must be increased. This is true because all other quantities besides \( \Delta H \) in the second term are normally positive. In the irradiated case, this is not always true, especially for \( \kappa_H \).
\[ \kappa_H = (1/H) \int_{0}^{\infty} \chi_\lambda H_\lambda^{\text{tot}} d\lambda < 0 \]

\[ \Delta H < 0 \]

Figure 1. A comparison between the total, extrinsic and intrinsic flux-weighted opacities measured at \( \tau_{\text{std}} = 1.0 \). The figure is for illustrative purposes only, and does not necessarily represent the conditions in a real atmosphere. In this situation, \( H < 0, \Delta H < 0 \) and \( \kappa_H < 0 \). When this occurs, a temperature correction will be generated in the wrong direction.

In the presence of a large extrinsic flux, the total flux (\( H_{\text{total}} = H_{\text{int}} + H_{\text{ext}} \)) may be negative since \( |H_{\text{ext}}| \gg H_{\text{int}} \) and \( H_{\text{ext}} < 0 \), which will lead to \( \Delta H < 0 \). In the case of cool secondaries, both the intrinsic flux and the opacities peak in the IR while the extrinsic flux peaks in the optical or ultra-violet. It is, therefore, possible that the total flux may be negative while \( \int_{0}^{\infty} (\kappa_\nu + \sigma_\nu) H_\nu d\nu \) is positive. A situation where \( H < 0, \Delta H < 0 \) and \( \kappa_H < 0 \) is illustrated in Figure 1. If this occurs, the second term on the right hand side of equation 12 will lead to corrections in the wrong direction causing instabilities.

The solution to this problem is straightforward if the following changes are considered. As was done for \( \Delta J \) and \( \Delta K \), \( \kappa_H H \) may be separated into intrinsic and extrinsic components:

\[ \kappa_H H = \kappa_H^{\text{int}} H_{\text{int}} + \kappa_H^{\text{ext}} H_{\text{ext}} \]  \hspace{1cm} (17)
where

\[ \kappa_{H}^{\text{int}} = \frac{1}{H_{\text{int}}} \int_{0}^{\infty} (\kappa_{\nu} + \sigma_{\nu}) H_{\nu}^{\text{int}} \, d\nu \]  

(18)

\[ \kappa_{H}^{\text{ext}} = \frac{1}{H_{\text{ext}}} \int_{0}^{\infty} (\kappa_{\nu} + \sigma_{\nu}) H_{\nu}^{\text{ext}} \, d\nu. \]  

(19)

It is also plausible to assume that \((\kappa_{H}^{\text{ext}} H_{\text{ext}}) \approx (\kappa_{H}^{\text{int}} H_{\text{int}})'\), in which case, the integrand in equation 12 becomes,

\[ \int_{0}^{\tau} q(\tau') \frac{\kappa_{H}^{\text{int}}(\tau')}{\kappa_{P}^{\text{ext}}(\tau')} \Delta H(\tau') \, d\tau', \]  

(20)

where \(\Delta H = H_{\text{int}} - H_{\text{target}}\). \(\kappa_{H}^{\text{int}}\) will always be positive (since \(H_{\text{int}} > 0\)), and the correction should be generated in the proper direction. Note that \(\kappa_{J}\) in the second equation of 8 could be reduced in a similar manner to \(\kappa_{J}^{\text{int}}\), however testing has shown that this usually does not lead to any major improvements.

On a practical note, when solving the radiative transfer equation, the entire radiation field is considered (intrinsic and extrinsic) and the total intensities are normally solved for. In order to implement the modifications introduced above, the radiative transfer equation must be solved twice per global iteration; once without the extrinsic radiation field and a second time with the extrinsic radiation. The difference between the monochromatic intensities with and without the extrinsic radiation gives the intrinsic intensities. Once the separate intensities are known, the separate moments of the radiation field may be calculated and the temperature corrections determined.

For \(\tau < 1\), the second correction term in Eq. 12 becomes more important with increasing external radiation and the modifications are crucial for the U-L procedure to work. For large external flux and an initial guess that is far from the correct structure (but reasonably close by most standards), the unmodified U-L scheme will produce large oscillating temperature corrections and usually will not converge while the modified scheme converges nicely (i.e. energy is conserved to the prescribed accuracy). Even when the correct solution is used as the initial guess, the unmodified scheme moves away from the correct solution and stabilizes on a different structure which doesn’t satisfy radiative equilibrium.

### 2.4. Global Iteration Scheme

As the first step in our outermost iteration loop (the “model iteration”) we use the current best guess of \(\{T, n_{i}\}\) as function of radius to solve the hydrostatic or hydrodynamic equations to calculate an improved run of \(P_{\text{gas}}\) with radius. Simultaneously, the population numbers are updated to account for changes in \(P_{\text{gas}}\). The next major step is the computation of the radiation field for each wavelength point (the “wavelength loop”), which has the prerequisite of a spectral line selection procedure for LTE background lines. Immediately after the radiation field at any given wavelength is known (note that the U-L procedure requires that the radiation field is consistent with the current opacities, so we
solve the radiative transfer equation for each wavelength point to account for scattering), the radiative rates and the rate operators are updated so that their calculation is finished after the last wavelength point. In the next steps, the population numbers are updated by solving the rate equations for each NLTE species and new electron densities are computed; this gives improved estimates for \( \{n_t\} \). The last part of the model iteration is the temperature correction scheme outlined above (using opacity averages etc. that were computed in the wavelength loop) which delivers an improved temperature structure. If the errors in the constraint equations are larger than a prescribed accuracy, the improved \( \{T, n_t\} \) are used in another model iteration. Using this scheme, about 10–20 model iterations are typically required to reach convergence to better than about 1% relative errors, depending on the quality of the initial guess of the independent variables and the complexity of the model.

3. Summary and Discussion

In this contribution we have described the generalization of the Unsöld-Lucy temperature correction scheme to allow model calculations for irradiated extrasolar giant planets and the expanding atmospheres of SNe, novae and stellar winds. The U-L scheme has the advantages of being extremely simple, requiring virtually no computer time or memory and still performing well enough to be used in practical applications. It is very useful in detailed NLTE model atmosphere calculations because it allows the use of powerful nested iteration schemes that reduce memory requirements and CPU time and that tend to increase numerical stability compared to more traditional approaches. However, no numerical method is perfect and care has to be taken to use the U-L scheme logically (see also Dreizler, this volume). One important factor is that it requires the radiation field to be consistent with the opacities, otherwise it cannot produce a usable temperature correction (i.e., standard ALI schemes will not work with an U-L type temperature correction without modification of the ALI scheme itself).

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References

Auer, L. H. 1971, JQSRT, 11, 573
Hauschildt, P. H. 1992, JQSRT, 47, 433
Hauschildt, P. H. 1993, JQSRT, 50, 301
Hauschildt, P. H., & Baron, E. 1999, Journal of Computational and Applied Mathematics, 102, 41
Unsöld, A. 1968, Physik der Sternatmosphären, 2nd edition (Heidelberg: Springer)