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ITERATION FACTORS IN THE LINE FORMATION PROBLEM WITH FREQUENCY DEPENDENT SOURCE FUNCTION

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SUMMARY: In this paper some iteration factors families introduced previously to solve the pure line transfer problem are generalized to the case when the background continuum is taken into account.The convergence properties of these factors are discussed when they are applied to the solution of the two-level atom line transfer problem in a constant and variable property media.

Key words. Radiative transfer, Line: formation, methods: numerical

1. INTRODUCTION

As a necessary step of many important astrophysical problems, NLTE line transfer problems are among the most difficult ones because of the nonlocal, and, in general, non-linear coupling between the radiation field and the excitation state of gas. Due to the complexity of these problems, there is still a great need for simple and efficient numerical schemes for their solution.

At present, the line transfer problems are mostly solved with the so called, Accelerated/Approximated Λ iteration (ALI) methods. They create a broad class of numerical schemes that employ certain approximations together with the operator perturbation technique in order to accelerate the simplest iterative procedure, the so called Λ iteration, that solves the radiative transfer (RT) and the statistical equilibrium equations (SE) in turn. The approximations can be physical (e.g. the core saturation assumption of Rybicki 1972) or numerical (e.g. the diagonal of the full Λ matrix (operator) of Olson et al. 1986). For the case of multi level radiative transfer problems, which are strongly nonlinear, ALI methods employ either linearization (e.g. Scharmer and Carlsson 1985) or introduce approximate Λ operators directly into the SE equations in order to make them linear (preconditioning), as is the case with Multilevel Accelerated Λ Iteration (MALI) method of Rybicki and Hummer (1991). A recent review of ALI methods was given in the paper of Hubeny (2003). Here, we shall point out the Forth-and-Back Implicit Λ Iteration (FBILI) method, an efficient method developed by Atanacković-Vukmanović, Crivellari and Simonneau (1997), whose solutions will be compared with those presented in this paper. By using the implicit representation of the source function in the computation of both incoming and outgoing radiation field intensities, that are treated separately within a forth and back approach, FBILI drastically accelerates the Λ iteration resulting in an extremely fast convergence to the exact solution. Its accuracy was checked for the case of two-level-atom line transfer problems with complete, as well as with partial frequency redistribution, and for the case of multilevel atom line formation problems with complete redistribution. Applied first to the NLTE radiative transfer problems in plane-parallel geometry, the FBILI method was generalized to spherically symmetric media in the paper by Atanacković-Vukmanović (2003).

In this paper we follow another approach, based on a simple iterative scheme that uses quasi-invariant functions, the so-called iteration factors, in order to speed up the most straightforward, but extremely slow, Λ iteration procedure. This is the Iteration Factors method (IFM). The idea of using the ratio of two moments of radiation field intensity in the stellar atmosphere model calculations appeared in the paper of Feautrier (1964), and was first applied by Auer and Mihalas (1970) in the form of the variable Eddington factor (K_ν/J_ν) for the solution of monochromatic transfer problem in plane-parallel geometry. The IF method is developed for solving the two-level atom line transfer problem by Atanacković-Vukmanović and Simonneau (1994) and extended to the more general multilevel atom problem by Kuzmanovska-Barandovska and Atanacković (2010). In the above cited papers the profile function is considered depth-independent. In the case of a variable-property medium or, more precisely, of a depth-dependent profile function, somewhat different definition of IFs families is required, as described in papers by Atanacković-Vukmanović and Simonneau (1993, 1995). The latter is hereinafter referred to as Paper I. Several iteration factors families were defined and their convergence properties analyzed when they were applied to the two-level atom line transfer with no background continuum. In this paper, a generalization is made to the case when the continuum is taken into account. We investigate the convergence properties of such a procedure considering both cases of a constant and depth dependent profile function.

2. ITERATION FACTORS

We shall proceed from the well known form of the RT equation for a static, plane-parallel medium:

$$\mu\frac{dI_{x\mu}(\tau)}{d\tau} = (\varphi_x(\tau)+\beta(\tau))(I_{x\mu}(\tau)-S_x(\tau)), \quad (1)$$

where φ_x is the absorption line profile, β denotes the ratio of continuum to the line opacity ($\beta = \chi^c/\chi^l$), $I_{x\mu}$ is the specific intensity of the radiation field at optical depth τ, x is the frequency displacement from the line center in Doppler width units and μ is the cosine of the angle between the photon path and the outward normal. The total source function $S_x(\tau)$ is given by:

$$S_x(\tau) = \frac{\varphi_x(\tau)}{\varphi_x(\tau)+\beta(\tau)}S^l(\tau) + \frac{\beta(\tau)}{\varphi_x(\tau)+\beta(\tau)}S^c(\tau) \quad (2)$$

where the line source function $S^l(\tau)$ is frequency independent for the case of complete redistribution and the continuum source function S^c is assumed to be equal to the Planck function $B(\tau)$.

For the two- level atom model $S^l(\tau)$ takes the form:

$$S^l(\tau) = \varepsilon B(\tau) + (1-\varepsilon)\int_{-\infty}^{\infty}\varphi_x(\tau)J_x(\tau)dx, \quad (3)$$

where $J_x(\tau)$ is the mean intensity of the radiation field and the standard non-LTE parameter ε represents the probability that the photons are thermalized by collisional deexcitation.

In the case of radiation transport by two-level atoms, the dependence of the line source function on its mean radiation field intensity is linear. The explicit form of the source function Eq. (3) enables a straightforward definition of the relevant intensity moments and the iteration factors as their ratios. The procedure using IFs is as follows: At the beginning of each iteration step the IFs are computed from the formal solution of the radiative transfer (RT) equation with the given (old) source function. They are then used to close the moments of the RT equation, whose solution gives the new and improved value of the source function.

In general, the absorption-line profile φ_x depends on the optical depth τ. As it was noted in Paper I, with respect to the case φ_x = const. the moment equations and the corresponding iteration factors families have to be defined in a different way. Following the procedure explained in Paper I we integrate Eq. (1) over angles by applying the operators $\int_{-1}^{1}..d\mu$ and $\int_{-1}^{1}..\mu d\mu$, and then perform the frequency integration within the range $[-x_N, x_N]$. This frequency interval has to be large enough as to include all the photons in the spectral line.

Since the integration over angles is performed on the interval [-1,1], the obtained intensity moments are considered "full". The system of moment equations containing the "full" angle and frequency integrated moments takes the form:

$$\frac{d}{d\tau}H = \beta(J-S) + (J_\varphi - S_\varphi), \quad (4a)$$

$$\frac{d}{d\tau}K = \beta H + H_\varphi, \quad (4b)$$

where the following notation is used:

$$Q(\tau) \equiv \int Q_x(\tau)dx$$

and

$$Q_\varphi(\tau) \equiv \int Q_x(\tau)\varphi_x(\tau)dx,$$

for the intensity and source function moments.

The system Eq. (4) is closed by means of three types of iteration factors families. The most straightforward factors (denoted as family A) include the generalized Eddington factor F, and the factors f_J and f_H that take into account the repartition of the energy over frequencies within the line profile:

$$F = \frac{K}{J_\varphi},\ f_J = \frac{J}{J_\varphi},\ f_H = \frac{H}{H_\varphi}. \tag{5}$$

In the second (B) family of IFs, the factors are defined so that the local, i.e. "passive in transfer" terms are isolated, and the iterations are performed only on the non-local ("active in transfer") terms of the radiation field. Hence, apart from the generalized factor F, the B-family contains $\tilde{f_J}$ and $\tilde{f_H}$ that are the ratios of only non-local parts of the corresponding intensity moments:

$$\tilde{f_J} = \frac{\tilde{J}}{\tilde{J_\varphi}} = \frac{J - (S - \frac{M_{12}}{2})}{J_\varphi - (S_\varphi - \frac{M_{22}}{2})},$$

$$\tilde{f_H} = \frac{\tilde{H}}{\tilde{H_\varphi}} = \frac{H - (S - \frac{M_{13}}{2})}{H_\varphi - (S_\varphi - \frac{M_{23}}{2})}, \tag{6}$$

where

$$M_{nm} = \int \varphi_x^{(n-1)}(\tau) S_x(\tau) dx \int \mu^{(m-2)} e^{-\tau(\varphi_x+\beta)\mu} d\mu.$$

The C-type factors take into account the non-local nature of the radiation field, but also two-point boundary nature of the RT process and the two-stream model of radiation field using the inward and outward intensity moments. Therefore, apart from the generalized Eddington factor F, this family consists of the following factors:

$$\alpha^+ = \frac{\beta(J^+ - S) + (J_\varphi^+ - S_\varphi)}{J_\varphi^+ - S_\varphi},$$

$$\alpha^- = \frac{\beta(J^- - (S - M_{12})) + J_\varphi^- - (S_\varphi - M_{22})}{J_\varphi^- - (S_\varphi - M_{22})},$$

$$\mu^+ = \frac{H^+ - \frac{S}{2}}{J_\varphi^+ - S_\varphi},$$

$$\mu^- = \frac{H^- - (\frac{S}{2} - M_{13})}{J_\varphi^- - (S_\varphi - M_{22})},$$

$$\Theta^+ = \frac{\beta(H^+ - \frac{S}{2}) + (H_\varphi^+ - \frac{S_\varphi}{2})}{H^+ - \frac{S}{2}},$$

$$\Theta^- = \frac{\beta(H^- - (\frac{S}{2} - M_{13})) + H_\varphi^- - (\frac{S_\varphi}{2} - M_{23})}{H^- - (\frac{S}{2} - M_{13})} \tag{7}$$

Another system of moment equations can be derived by using the two-stream model of radiation field. The outgoing $I_{x\mu}^+$ and incoming $I_{x\mu}^-$ intensities and the corresponding moments are treated separately. By performing the μ-integration on the intervals [-1,0] and [0,1] and then the frequency integration applying $\int_{-x_N}^{x_N} dx$, the system takes the form:

$$+\frac{d}{d\tau} H^+ = \beta(J^+ - S) + (J_\varphi^+ - S_\varphi), \tag{8a}$$

$$-\frac{d}{d\tau} H^- = \beta(J^- - S) + (J_\varphi^- - S_\varphi). \tag{8b}$$

The forth family (D) of factors we consider here is used to close the system Eq. (8) of moment equations. The factors are defined as the ratios of two-stream intensity moments:

$$\alpha^\pm = \frac{J^\pm}{J_\varphi^\pm},\ \Theta^\pm = \frac{H^\pm}{J_\varphi^\pm}. \tag{9}$$

Being angle and frequency integrated, the iteration factors reduce the numerical description of the problem to only two scalar moment equations. Hence, the system Eq. (4) is transformed into the following form:

$$\frac{d}{d\tau} H = E_{11} H + E_{12} K + V_1, \tag{10a}$$

$$\frac{d}{d\tau} K = E_{21} H + E_{22} K + V_2, \tag{10b}$$

and solved for the unknown moments K and H. Let us note that the coefficients E_{ij} and V_i depend on the chosen iteration factors family (A, B or C). Similarly, by the use of D family, system Eq. (8) is transformed into two moment equations containing the unknown moments H^+ and H^-:

$$\frac{d}{d\tau} H^+ = G_{11} H^+ + G_{12} H^- + W_1, \tag{11a}$$

$$\frac{d}{d\tau} H^- = G_{21} H^- + G_{22} H^+ + W_2, \tag{11b}$$

where the known iteration factors are contained in the coefficients G_{ij} and W_i. The solutions of the systems Eq. (10) and Eq. (11) are used in the computation of the improved values of J_φ and the new values of the source function that enter the next iteration step. In order to achieve fast convergence to the exact solution, the iteration factors have to be nearly independent from the initial solution.

3. CONVERGENCE PROPERTIES

In order to test the convergence properties of the four families of iteration factors we solved the problem of spectral line formation in a semi infinite atmosphere with $\epsilon = 10^{-4}$ and $\beta = 10^{-3}$ and for two cases: a) $B = 1$ (Case 1) and b) $B = B(\tau)$ (Case 2). For the sake of simplicity we assume pure Doppler broadening so that the absorption line profile φ_x is defined by a Gauss normalized profile function:

$$\varphi_x(\tau) = \frac{1}{\sqrt{\pi}\delta(\tau)} e^{-x^2/\delta(\tau)^2}, \tag{12}$$

where $x = (\nu - \nu_0)/\Delta\nu_D^*$ is the frequency displacement from the line center. It is expressed in fixed frequency units $\Delta\nu_D^*$ equal to Doppler width at great optical depths. The parameter $\delta(\tau)$ is given by:

$$\delta(\tau) = \frac{\Delta\nu_D(\tau)}{\Delta\nu_D^*}. \tag{13}$$

First, we assumed that φ_x is depth independent ($\delta = 1$) throughout the atmosphere since the analytical solutions for that case are known. Then, we consider the general case of variable $\varphi_x(\tau)$.

The properties of the iterative procedure were analyzed by means of three quantities (Auer et al. 1994) computed at each iteration step i:

$$R_c^i = \left| \frac{S^i - S^{i-1}}{S^i} \right|_{\max}, \tag{14}$$

$$C_e^i = \left| \frac{S^i - S^\infty}{S^\infty} \right|_{\max}, \tag{15}$$

$$T_e^i = \left| \frac{S^i - S^\infty_{\mathrm{FBILI}}}{S^\infty_{\mathrm{FBILI}}} \right|_{\max}. \tag{16}$$

Here, R_c is the maximum relative change, C_e is the maximum relative convergence error, and T_e is the maximum relative true error, while S^∞ and S^∞_{FBILI} are the fully converged solutions obtained by a preliminary long run with the IFM and the FBILI method, respectively. The latter was used as the reference code so that we expressed the true accuracy of the IFM solutions with respect to the solutions obtained with the FBILI method using the same discretization in angles, frequencies, and optical depths.

The iterative procedure converged rapidly for all four families of factors, reaching the maximum relative correction R_c of about 10^{-5} for Case 1. As expected, the convergence properties of various families are highly influenced by the degree of sophistication in their description of the physics of RT process. This is illustrated in Table 1 where the number of iterations needed to reach different values of maximum relative change R_c for all types of factors and for both Case 1 and Case 2 is given. Using the most straightforward A family of factors the usual convergence criterion $R_c \leq 10^{-2}$ was fulfilled in 17 and 20 iterations for the Case 1 and Case 2, respectively, while the convergence error of 1% (a measure of the internal accuracy) is reached in 26 and 35 iterations (see Table 2). When we iterate on "active in transfer" terms of radiation field (type B factors) only 11 and 14 iterations were needed, for two cases respectively, to reach the maximum relative correction of 1%, and 16 and 24 iterations to reach the convergence error of 1%. However, some instabilities may occur due to small (or null) divisors. This can be noticed in Fig. 1 where the variation of R_c, T_e and C_e with the iteration number for Case 1 and four types of iteration factors is presented. We can see in the graph for type B factors that although the procedure reaches $R_c \leq 10^{-5}$ for Case 1, the instabilities start at the very beginning of the iterative procedure. Fig. 2 shows the variation of R_c, T_e and C_e with the iteration number for Case 2 and four IFs families. Because of the instabilities the procedure using B-type IFs can not reach the maximum relative correction of 10^{-4} in this case.

Table 1. The number of iterations needed to achieve the convergence for four iteration factors families (A - D) and $B = 1$ (Case 1) and $B = B(\tau)$ (Case 2). Constant profile function is assumed.

R_c	Type A	Type B	Type C	Type D
	Case 1			
10^{-2}	17	11	11	8
10^{-3}	29	28	17	12
10^{-4}	44	40	26	14
10^{-5}	59	59	36	19
	Case 2			
10^{-2}	20	14	13	10
10^{-3}	37	33	25	14
10^{-4}	56	/	40	20
10^{-5}	76	/	57	24

Table 2. The number of iterations needed to achieve various convergence criteria for four iteration factors families and $B = 1$ (Case 1) and $B = B(\tau)$ (Case 2). Constant profile function is assumed.

	Type A	Type B	Type C	Type D
	Case 1			
$C_e < 10^{-2}$	26	16	13	8
$R_c < 0.1T_e(\infty)$	26	28	19	12
$C_e < 10^{-4}$	53	52	30	15
	Case 2			
$C_e < 10^{-2}$	35	24	20	10
$R_c < 0.1T_e(\infty)$	32	27	21	15
$C_e < 10^{-4}$	69	/	51	21

The best results were obtained by the use of the most refined, C and D families of iteration factors. Their definition takes into account the two-stream model of radiation field. This results in a rapid convergence to the exact solution already in the first few iterations. By the use of type C factors, 11 and 13 iterations were needed (for Case 1 and Case 2, respectively) to reach R_c of 1%, while C_e of 1% was reached in 13 and 20 iterations. With the use of more "simple" D family that closes the

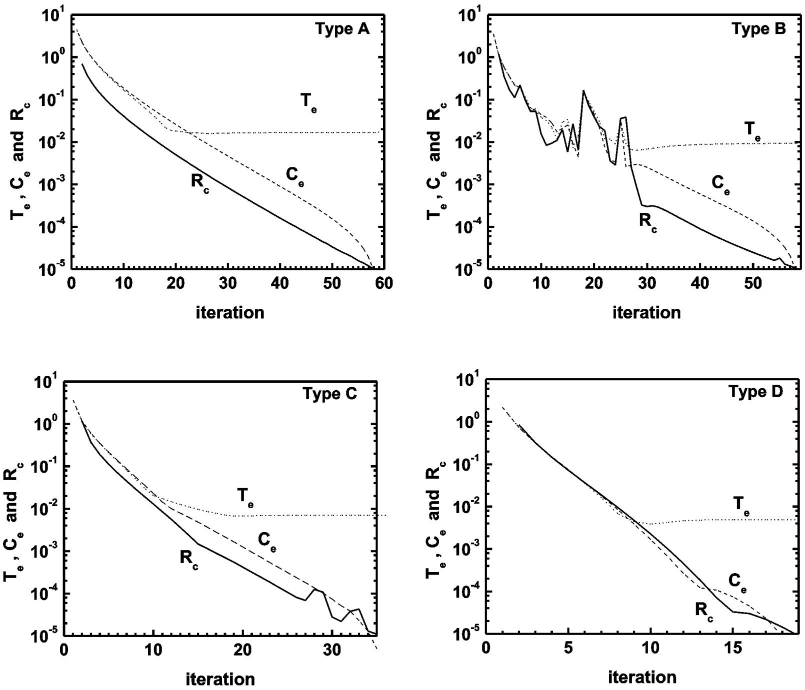

Fig. 1. *The maximum relative change R_c, the maximum relative convergence error C_e and the maximum relative true error T_e for four iteration factors families as a function of the iteration number for B=1.*

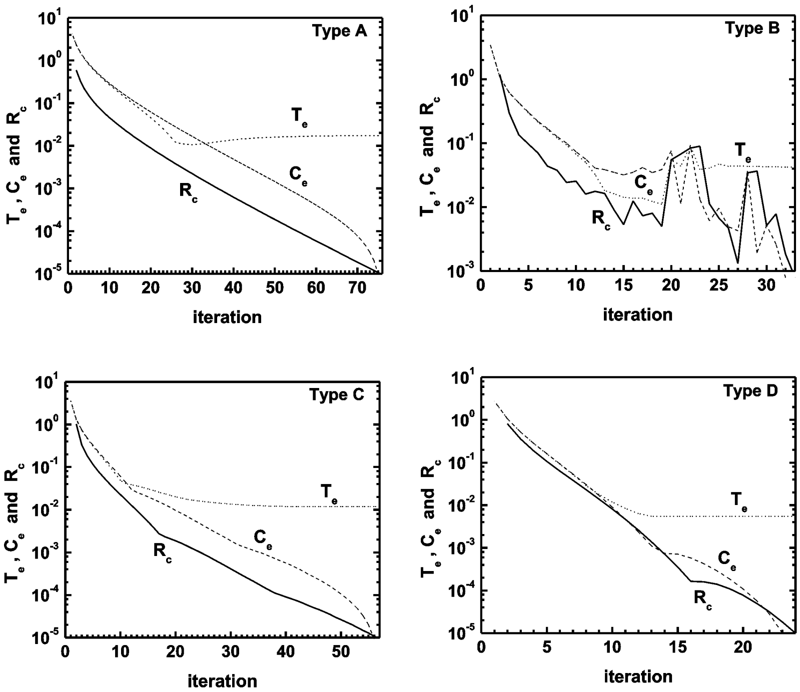

Fig. 2. *The maximum relative change R_c, the maximum relative convergence error C_e and the maximum relative true error T_e for four IF families as a function of the iteration number for $B = B(\tau)$.*

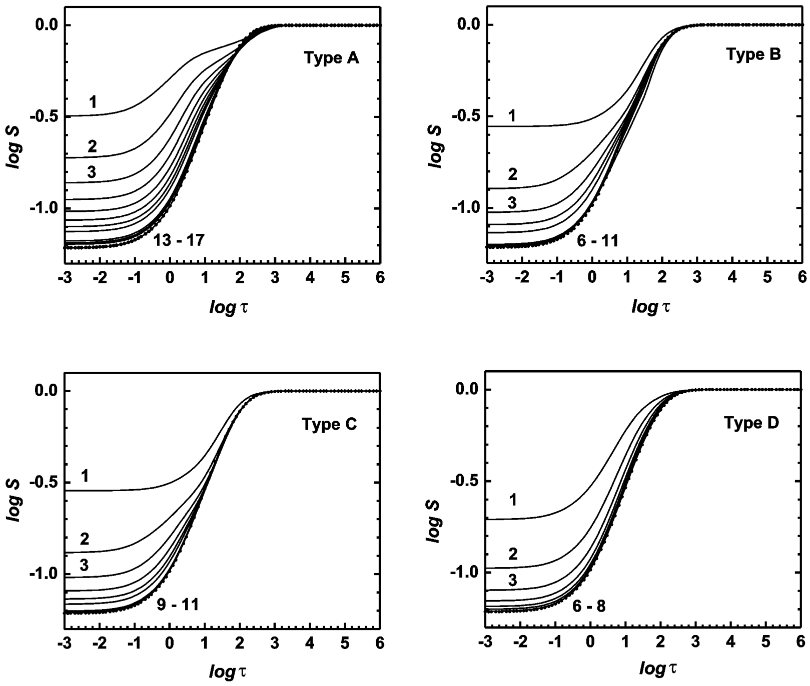

Fig. 3. *The source function after the indicated number of iterations (for the convergence criterium $R_c \leq 10^{-2}$) for four iteration factors families and B=1. The solutions obtained with FBILI are given by dots.*

system of two-stream moments (Eq. 8), both criteria: $R_c \leq 10^{-2}$ and $C_e \leq 10^{-2}$ were fulfilled in only 8 and 10 iterations, for two cases, respectively.

By analyzing Figs. 1 and 2, we can notice the very same behavior of the maximum relative true error T_e as that described in the paper by Kuzmanovska-Barandovska and Atanacković (2010). After a rapid initial improvement in the first few iterations, T_e reaches an asymptotic value, or the so-called truncation error $T_e(\infty)$, which is about 2 % for A-type factors, about 1% for B and C-type factors and less than 0.5% for D-type factors. The truncation error is a measure of the true accuracy since a further decrease in R_c does not improve the accuracy already achieved. Thus, it can be used to specify another stopping (convergence) criterion: $R_c < 0.1T_e(\infty)$, as was suggested by Auer et al (1994). The number of iterations, for the four families of iteration factors and for Case 1 and Case 2, needed to reach this criterion, as well as the criteria $C_e < 10^{-2}$ and $C_e < 10^{-4}$, is shown in Table 2.

In Fig. 3 we show the variation of the source function with optical depth in the run of iterations for the four families of iteration factors and Case 1, together with the solutions obtained with the FBILI method. The convergence criterion $R_c \leq 10^{-2}$ is used. We can see that the solution attains good thermalization depth already in the first iteration and the exact values of the source functions are achieved after just a few iterations. This is the important difference of the IFM with respect to the simple Λ iteration procedure. Namely, Λ iteration converges extremely slow by to a solution that thermalizes much higher in the atmosphere because it transfers more than necessary information from one part of an iterative step to the other. On the other hand, due to the use of iteration factors that get almost exact values already in the first iteration, the solutions are corrected simultaneously throughout the whole medium enabling a fast and stable convergence. The best convergence properties, the most exact and most rapid solutions are obtained with the D-type iteration factors. The true accuracy of less than 0.5% is reached in only 8 iterations. The behavior over iterations of these factors is shown in Fig. 4.

Further tests of the IF families described above are performed by solving linear line transfer problem with depth-dependent profile function. For the case of pure Doppler broadening, the depth variation of φ_x is expressed via the depth variation of the Doppler width $\Delta\nu_D(\tau)$. Here, we used depth variation of $\Delta\nu_D(\tau)$ in the form proposed by Rybicki and Hummer (1967). Two cases that define "cool" and "hot" surface layers, respectively, were considered:

$$\Delta\nu_D(\tau) = 2 - e^{-A\tau}, \tag{17a}$$

$$\Delta\nu_D(\tau) = 1 + e^{-A\tau}. \tag{17b}$$

Again, we assumed the line formation in a semi-infinite medium with $\varepsilon = 10^{-4}$ and $\beta = 10^{-3}$.

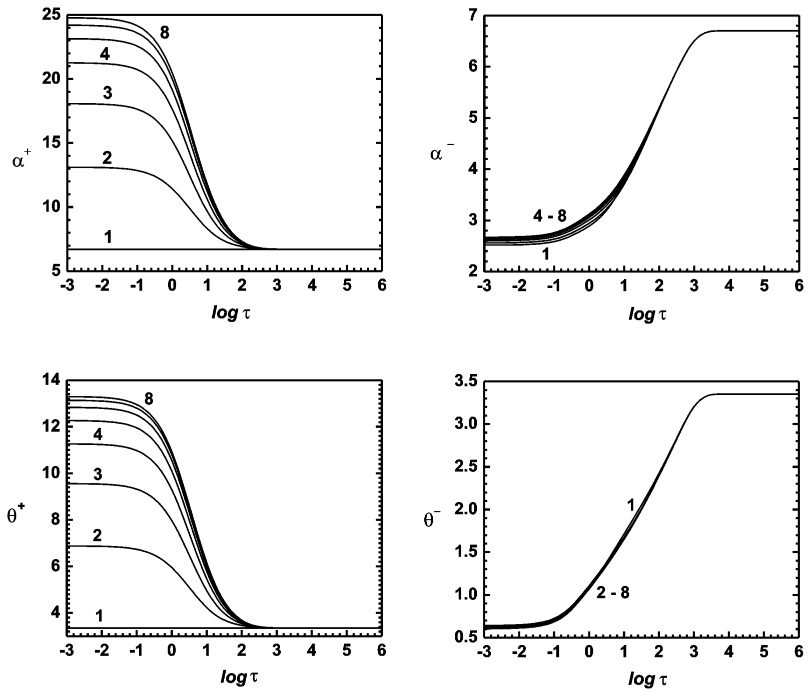

Fig. 4. *Variation of the D- type factors over the iterations for B=1.*

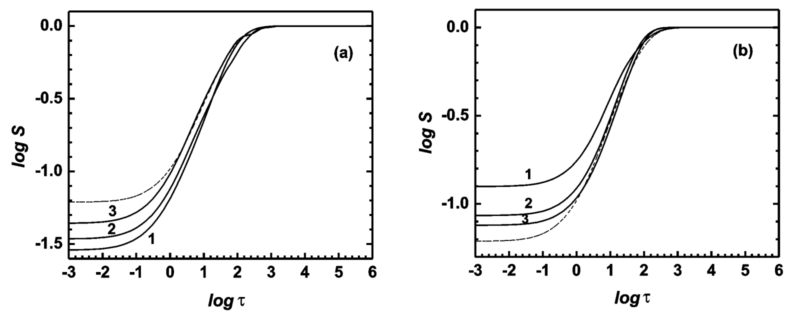

Fig. 5. *The source functions in variable property media: (a) "Cool" surface layer, (b) "Hot" surface layer. Curves labeled by $n = 1, 2, 3$ correspond to different values of coefficient $A = 10^{-n}$. The solutions for $\delta = 1$ are given by dashed lines.*

The tests proved that the convergence properties of four IFs families for the case of depth-dependent profile function are similar to the ones for constant profile function ($\delta = 1$). Again, the best results were obtained with D-type factors. In Table 3 we show the number of iterations necessary to achieve different maximum relative corrections for "cool" and "hot" surface layers. Three different values of the coefficient $A = 10^{-1}, 10^{-2}$ and 10^{-3} were considered. The usual convergence criterion $R_c \leq 10^{-2}$ was fulfilled in 15, 18 and 18 iterations for "cool" surface layer, and for three values of A, respectively, and in 7, 5 and 4 iterations for the respective values of A but for the "hot" surface layer. With regard to 8 iterations needed to achieve the same criterion for the case of constant profile function, the results are as expected. For the "cool" surface layer the profile φ_x is much narrower and the increase of $\Delta\nu_D$ grows deeper in the medium requiring more iterations with respect to the $\delta = 1$ case. On the other hand, for the "hot" surface layer the absorption profile is wider and the convergence is achieved in smaller number of iterations. The source functions for two cases defined in Eq. (17) and three values of the coefficient A (with the convergence criterion $R_c \leq 10^{-2}$) are presented in Fig. 5.

Table 3. The number of iterations needed to achieve the convergence for the D-type iteration factors and "cool" and "hot" surface layer.

"Cool" surface layer			
R_c	$A = 10^{-1}$	$A = 10^{-2}$	$A = 10^{-3}$
10^{-2}	15	18	18
10^{-3}	24	29	27
10^{-4}	33	39	38
10^{-5}	41	47	55
"Hot" surface layer			
R_c	$A = 10^{-1}$	$A = 10^{-2}$	$A = 10^{-3}$
10^{-2}	7	5	4
10^{-3}	11	7	5
10^{-4}	15	9	7
10^{-5}	19	12	10

4. CONCLUSION

In this paper several families of iteration factors are used to solve the two-level atom line formation problem when the spectral line is superposed to the background continuum. A simple test case of a spectral line formed by Doppler broadening in a semi-infinite atmosphere with $\varepsilon = 10^{-4}$ and $\beta = 10^{-3}$ is solved. The cases of constant and depth-dependent profile function are considered. The iteration factors, computed at the beginning of each iteration from the formal solution of the RT equation, are used to close two systems of RT moment equations. One system is derived by performing the integration over all angles, whereas the other system is obtained by using the two-stream model of the radiation field; the both are integrated over all line frequencies.

By analyzing the convergence properties of four families of iteration factors (A, B, C, D) we can conclude that their use in the case of depth-independent profile function leads to a rapid and stable convergence to the solutions that differ by only 0.4-2% from the solutions obtained by the reference FBILI method. Only 10-30 iterations are needed to fulfill various convergence (stopping) criteria. This is less than in the pure line transfer case described in Paper I since, by adding the continuum opacity, the thermalization length decreases, thus making the conditions of line formation closer to LTE. The procedure also converged very fast for all IFs families when the case of depth-dependent profile function was considered. The best convergence properties are obtained using D-type factors confirming again the fact that the IFs, more related to the physics of the problem, lead to faster and more stable convergence.

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ИТЕРАЦИОНИ ФАКТОРИ У ПРОБЛЕМУ ФОРМИРАЊА ЛИНИЈА СА ФРЕКВЕНЦИОНО ЗАВИСНОМ ФУНКЦИЈОМ ИЗВОРА

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Оригинални научни рад

У овом раду је употреба неколико претходно дефинисаних фамилија итерационих фактора уопштена на случај формирања линија када се узме у обзир континуум на који належу или су суперпониране линије. Дискутована су конвергентна својства итеративне процедуре примењене на решење проблема формирања линија за модел атома са два нивоа у срединама константних и промењљивих својстава.