Determination of C, N, and O abundances in the atmospheres of late-type stars. Extreme value problem

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The possibility of determining carbon, nitrogen, and oxygen abundances by solving an extreme value problem is shown. The functional to be minimized is constructed from differences between the observed and calculated characteristics of atomic and molecular lines or their blends. A brief description of the procedure and the results of a determination of C, N, and O abundances in the atmosphere of a K giant is given.

At the temperatures and densities of matter typical of the atmospheres of late-type stars, a considerable number of carbon, nitrogen, and oxygen atoms are bound into molecules. Chemical equilibrium in their atmospheres is controlled, on the whole, by the quantity C/O = ε(C)/ε(O). Here and below, ε(x) is the abundance of element x on the scale \( \sum x = 1.0. \)

There are no intense nitrogen or carbon absorption lines in the spectra of late-type stars. In determining the C, N, and O abundances in the atmospheres ..., a line has been lost from the Russian text ..., as well as the 630.03 and 636.3 nm lines of neutral oxygen. The intensity of absorption lines of a molecule that incorporates oxygen, nitrogen, or carbon atoms depends in a complex way on the abundances of these elements in the stellar atmosphere. A fixed equivalent width of an absorption line of such a molecule in the three-dimensional space with coordinates ε(C), ε(N), and ε(O) corresponds to a set of values of the C, N, and O abundances, which can be represented in the form of a certain curve: the line of equal equivalent width (LEEW). For absorption lines of different molecules, the LEEWs intersect a part of the space whose volume is determined by the total errors of the observations and calculations. The LEEW method has been used traditionally to determine the C, N, and O abundances in the atmospheres of cool stars (see Ref. 1). Since this method is fairly laborious, searches have continued for less unwieldy ways of determining the abundances of those elements. It is possible to determine the analytical dependence of the characteristics (equivalent widths or central intensities) of molecular absorption lines on the C, N, and O abundances only within the framework of the simplest concepts of their production in stellar atmospheres. Kjergaard et al. have used such dependences only to estimate the errors of the LEEW method.

In the present paper we describe an algorithm for determining C, N, and O abundances in the atmospheres of late-type stars by minimizing functionals comprised of the differences between observed and calculated characteristics of absorption lines. Suppose that \( K \) equivalent widths of absorption lines of oxygen and of molecules whose composition includes C, N, or O atoms have been obtained from observations. We can write the following system of nonlinear equations:

\[
\text{abs}(W_k^{\text{obs}} - W_k^{\text{bl}}) = F_k[\varepsilon(C), \varepsilon(N), \varepsilon(O)],
\]

\[ k = 1, \ldots, K. \] (1)

Here \( W_k^{\text{obs}} \) and \( W_k^{\text{bl}} \) are the observed and calculated equivalent widths of the \( k \)th absorption line.

The determination of the C, N, and O abundances for which the abs(\( W_k^{\text{obs}} - W_k^{\text{bl}} \)) are smallest, i.e., \( \partial F_k/\partial \varepsilon = 0, \) \( k = 1, \ldots, K, \) is an example of an extreme value problem. We use Newton's method (see Ref. 3) to solve the system of equations (1). For the zeroth approximation, we can use the C, N, and O abundances in the solar atmosphere or their characteristic mean values for stars of similar spectral types. We obtain the next approximation from the solution of the system of linear equations

\[
F_k + \sum_j A_{kj}(\varepsilon_{j,1} - \varepsilon_{j,1}) = 0, \quad k = 1, \ldots, K, \] (2)

where \( \varepsilon_{j,1} \) is the abundance of the \( j \)th element at the \( 1 \)th step of the iteration process, \( J \) is the total number of unknowns, and

\[
A_{kj} = \frac{\partial F_k}{\partial \varepsilon_{j,1}} \approx \frac{F_k(\varepsilon_{j,1} + \delta \varepsilon_j) - F_k(\varepsilon_{j,1})}{\delta \varepsilon_j}. \] (3)

If \( K > J \), system (2) can be solved by the least squares method. The C, N, and O abundances being sought are found after a few iterations. Absorption lines that are parts of blends can also be used to solve system (1).

The above algorithm for determining C, N, and O abundances has been implemented in the form of the ABEL6 program. Individual subroutines were taken from SAM71, a modification of the SAM1 program. We made the following changes in our version of the program for calculating model atmospheres (SAM71): a) the radiative transport equation is solved by Hermite's method; b) the possible number of depths in the model atmosphere has been increased to 71; c) the possible number of atoms, ions, and molecules that can be taken into account in calculating dissociative-ionization...
oscillator strengths of lines of other atoms and molecules that make up these blends.

The algorithm for determining C, N, and O abundances by minimizing $\Phi_k$ was implemented in the form of the ABEL7 program.

The results of determinations of abundances by means of the ABEL6 and ABEL7 programs for absorption lines with reliably determined characteristics ($r_k$ and $W_k$) should coincide. This assumption was tested by direct calculations.

The ABEL6 program was used to calculate the central intensities of the O I 630.0 and 636.3 nm and C2 513.5 nm absorption lines for a model atmosphere of \( \rho \) Boo with oxygen and carbon abundances $-3.42$ dex and $-3.82$ dex, respectively. For these values of \( e(C) \) and \( e(O) \), the theoretical equivalent widths correspond to the observed ones. Instrumental broadening was taken into account in calculating the absorption line profiles. The instrumental profile was a Gaussian with a halfwidth 0.18 Å. The central intensities of O I and C2 lines thus calculated were specified as $r_k^{\text{obs}}$ in determining the O and C abundances in the atmosphere of \( \rho \) Boo using the ABEL7 program. The initial values $e_0(C)$ and $e_0(O)$ were the same as those used earlier (see Fig. 1).

The resulting C and O abundances coincided with the ABEL6 results. An analysis of the numerical calculations showed that the convergence of the iteration process in the solution of system (4) practically coincides with that shown in Fig. 1. The maximum differences in O and C abundances in an individual step of the iteration process did not exceed 5%. It must be noted, however, that this is possible only when unblended absorption lines or blends formed by lines of the same molecule, which occurred in the case described above, are used to determine the C, N, and O abundances. Our experience with numerical calculations shows that when more complicated blends are used, which include absorption lines of many atoms and molecules, the convergence process is more stable in the solution of system (1) than in the solution of system (4).

The use of both versions of the procedure requires a relatively large number of calculations. In each iteration, one calculates $J + 1$ states of ionization-dissociative equilibrium and $K(J+1)$ sections of synthetic spectrum. Here, as before, $J$ is the number of abundances being determined and $K$ is the number of spectral features. Our experience shows that it is advisable to use the procedures described above on a computer with an operating speed of at least 10^6 operations/sec. The results given in Fig. 1 were obtained in ~200 min on an ES 1060 computer.

We note the advantages of such an approach in determining C, N, and O abundances in the atmospheres of cool stars.

1. For $K > J$, the influence of random errors in the oscillator strengths and errors in measuring the characteristics of the absorption lines, which are always present in work of this kind, is reduced (strictly in the least squares sense).

2. The number of routine calculations of the characteristics of the absorption lines and of their subsequent human analysis is reduced to a minimum. The search for a solution is optimized in a certain sense.

3. In the LEEW method, lines of some molecules are used to determine the C and O abundances and lines of other molecules are used to determine the N abundance. In the