MODEL ATMOSPHERES AND CHEMISTRY

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ABSTRACT. The limitations imposed on the accuracy of the abundance determination by the current status of the stellar atmosphere models are discussed. It is shown that the very high S/N ratio and resolution in spectroscopic observations require the new additional steps in stellar atmosphere modeling and in the line formation theory.

INTRODUCTION

First of all some introductionary remarks. After dr. Baschek's report I have changed my initial object therefore I shall tell very shortly about the observational accuracy of the abundance determination and shall make an accent on theoretical and computational limitations imposed by present status of stellar spectral line and stellar atmosphere modeling. In other words, I shall try to answer the question: Is this present status of modeling good enough to satisfy the observational accuracy of abundance determination?

"OBSERVATIONAL" ACCURACY OF ABUNDANCE DETERMINATIONS

In this part I only give an information additional to the excellent review by dr. Baschek. Table 1 contains some examples of recent abundance determinations: column 1 is the type of stars; column 2 - references; column 3 - the S/N ratio; column 4 - the resolution R or $\Delta\lambda$(Å); columns 5-7 are the errors in determination of T_{eff}, log g and turbulent velocity ξ_{turb}; columns 8-10 are the accuracy of abundance determinations (index) introduced by errors in T_{eff}, log g and ξ_{turb}; column 11 - combined errors; column 12 - the total accuracy in abundance determinations; column 13 - number of stars.

Column 12 of this table showed that overall accuracy of the abundance determination lies in interval (±0.05) ÷ (±0.3) dex. For cool stars the

G. Michaud and A. Tutukov (eds.), Evolution of Stars: The Photospheric Abundance Connection, 49–61.

TABLE 1

Stars	Reference	S/N	Resolution	ΔT_{eff}	$\Delta\log g$	Δv_{turb}	$f(\Delta T)$	$f(\Delta\log g)$	$f(\Delta v_{turb})$	$f(\Delta T, \Delta\log g, \Delta v_{turb})$	total	N stars
early type A	1			±200	±0.2		±0.15					17
stars	2			±150	±0.2	±0.5	±0.15	±0.09	±0.10		±0.22	1
	3			±250	±0.2						±0.23	4
B	4			±400	±0.11					±0.10+±0.30		
	5			+500	+0.5		+0.3	+0.16				9
wd	6			±500+±10000							±0.6+±1.0	2
	7			±500	±0.4						±0.5	1
	8		0.3	±1000	±0.2	±5.0	±0.2	±0.1	±0.3	±0.2	±0.3	4
Galactic	9	150	0.21	±50			±0.039				±0.05	44
cluster	10	45	0.2	±90			±0.18					7
	11	200	0.2	±200	±0.4	±0.5	±0.20	±0.01	±0.13		±0.13	53
	12	700	0.2	1-2%						±0.27	±0.27	25
	13	400	0.03	±100			±0.06					6
	14	200	20000	±80	±0.3	±0.3	±0.08	±0.03	±0.03		±0.08	24
	15	300	0.12	±150	±0.3	±0.2					±0.2	56
	16	265	0.21	±250							±0.07	33
halo stars	17	35	0.2	±200	±0.3	±0.5				±0.2	±0.2	36
	18		0.25	±110							±0.10+±0.33	54
	19	>200	100000	±100	±0.25	+0.3	+0.26	+0.17	-0.27		±0.20	1
	20	150		±100	±0.2		±0.09	±0.00				32
	21	>100		±100	±0.3	-0.5	+0.06	-0.14	+0.13		±0.15	20
	22	>150	0.26	±100		±0.5	±0.1		±0.05		±0.15	35
metal poor	23	200	0.3	±100	±0.30	±0.5	±0.14	±0.24	±0.16			13
stars	24	200	0.12	±100	-0.5	±0.5	+0.06	±0.36	-0.06	±0.01+±0.24	±0.06	25
	25	220	25000	±80	±0.5	±0.5	±0.12	±0.17	±0.04		±0.23	30
disk stars	26	200	0.13	±200			±0.1					24
	27	400	0.14	±100		±0.5	±0.1		±0.05		±0.2	13
	28			±100	±0.3		±0.1				±0.3	
	29	180	100000	±100	±0.5	±0.5	±0.08	±0.10	±0.05		±0.15	23
	30	100	0.2	±100	±0.3						±0.2	7
G-K dwarfs,	31	480	0.13	±100	±0.20		±0.10	±0.10			±0.09	4
supergiants										±0.2		
M giants	32			±100	±0.5						±0.22	20
variable	33		0.1	±200	±0.3	±0.5					±0.2	9
supergiants												

accuracy is higher ($\Delta\log\varepsilon < 0.1$), but for hot stars the accuracy is not better than ±0.2 dex.

We should not consider these numbers as a starting point for people modeling atmospheres, because the overall errors (see column 12) may originate from different sources. First, the limitations in the S/N and R values give the "pure observational errors" of the order $\Delta\log\varepsilon \approx \pm 0.05$ (see, for example [34]), at least, for cool stars. Second, the uncertainties in T_{eff} and log *g* give the "pure model errors". Third, I dare say that there is another source of errors which I call "personal".

"PERSONAL ERRORS" OF ABUNDANCE DETERMINATIONS

By the words "personal errors" I mean errors which may be introduced by preference of each spectroscopist to use one type of model atmospheres instead of others. Moreover, each of us prefers to use his own computing code instead of finding misprints in published codes.

Up to now the large number of model atmospheres has been published. This number is more than 5000. Among them the most popular are the models by Gustafsson et al. [35], Johnson et al. [36], Peytremann [37] for cool stars. For hot stars spectroscopists prefer to apply the NLTE models [38]. And without doubt the most cited author is R.Kurucz [39] who made many modeling people unemployed.

What is the influence of special choice of models on the abundance determinations? The clear answer to this question may be found in the paper by Villada et al. [40]. These authors have applied different model atmospheres for the abundance determination. Numerical experiments showed that the models of different authors may produce the error not more than $\overline{\Delta\log\varepsilon} = \pm 0.03$.

The following conclusion has been derived by authors: "We should rely more on the present status of the model atmosphere since even if there are discrepancies among models computed with different codes, these do not affect significantly the chemical abundance determination". I may say that this citation is true if one bear in mind that the authors really compared the different codes but not different input physics (LTE or NLTE, for example).

At present there are many different codes for the abundance determinations: WIDTH5, WIDTH6, LINFOR...- in the West, LINE, KONTOUR, SYNTHES...- in the USSR. My own experience has shown that there is no need to trouble about the identity of the abundance results taken by different codes, at least, for cool stars.

But for hot stars some caution would be necessary. In this connection I shall refer to the paper by Leushin and Topil'skaya [41]. Using different codes WIDTH5, WIDTH6 and KONTOUR, they computed theoretical equivalent widths for T_{eff} interval 8850 K - 22500 K. The results are shown in figure 1.

It is clear from figure 1a that there are no large differences in W_λ *for weak* lines. The abundance averaged over many lines of a chemical

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element is the same for the codes WIDTH6 and KONTOUR. The code WIDTH5

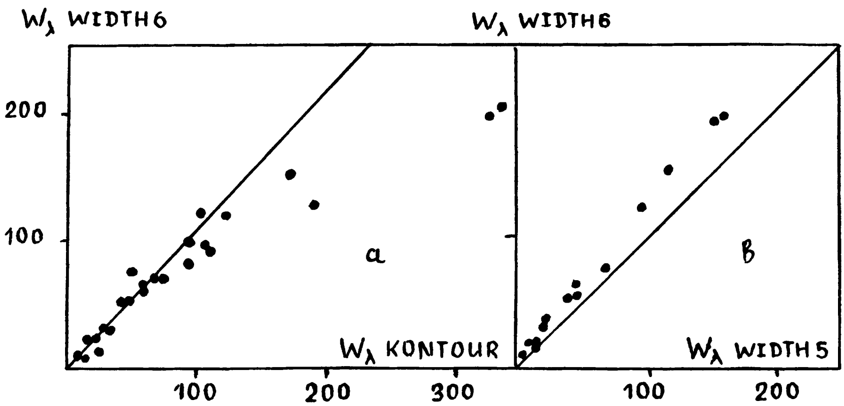


Figure 1. Comparison of the equivalent widths W_λ for different codes.

(figure 1b) gives systematically lower values W_λ. This may involve the error $\Delta\log\,\varepsilon = 0.3 \div 0.5$ in comparison with results according to the codes WIDTH6 or KONTOUR. Both figures convince us that the use of *strong* lines for the abundance determinations is not desirable: due to different treating of line broadening in different codes the results may not be selfconsistent. We should take care of *all* lines if the code WIDTH5 is used and of strong lines if the code WIDTH6 is used.

Having collected all the numbers $\Delta\log\,\varepsilon$ above mentioned, we argue that the theory of model atmospheres must provide the accuracy of the abundance determinations $\Delta\log\,\varepsilon$ not less ±0.1 - for cool stars and ±0.2 - for hot stars. This is the starting value for next discussion.

BASIC ASSUMPTIONS OF MODEL ATMOSPHERE THEORY

Basic conceptions of stellar atmosphere modeling have changed a little since the time of Milne:

- lateral homogeneity;
- plane-parallel structure;
- hydrostatic equilibrium with negligible change in gravity with depth;
- transfer of energy is due to radiation/convection;
- the atomic abundances are specified and assumed to be constant throughout the atmosphere;
- electrons are in thermal equilibrium because there are very frequent electron-electron collisions;
- level populations also are in thermal equilibrium (a priori!).

It is clear that these assumptions have been introduced just for the sake of convenience and simplicity of practical computations. My optimistic point of view that at present our level of knowledge and ability allows the modeling people to claim: "No more assumptions for us - we calculate!" Recent steps in the stellar atmosphere theory prove this statement. There are some examples below.

A few years ago the lateral homogeneity assumption has been criticized mainly in theoretical way. But recently Nordlund and Dravins [42-47] used the experience of *solar* granulation modeling and attempted a modeling of *stellar* granulation. The authors have solved the equations of three-dimensional and time-dependent hydrodynamics, coupled to those of three-dimensional non-grey radiative transfer for simulation volume of 32*32*32 elements, extending from inside a star through photosphere. These papers contain a great number of very important conclusions which could not be predicted by classical models. Some of them are concerned with the abundance determination problem.

It is the traditional way for the abundance determination to introduce freely adjustable parameter ξ_{turb} in spectral line calculations to have an agreement with observations. This value is used without much concern with it's real physical origin. But new hydrodynamic models give a good agreement with FeI line observations, and no fitting parameter is needed (!). Unfortunately the authors did not estimate numerically the influence of this fact on the values $\Delta\log\varepsilon$. By intuition we may guess that $\Delta\log\varepsilon$ must not be less than $(\pm0.2) \div (\pm0.3)$.

New models have shown also that homogeneous "classical" models may give wrong abundances in principle. The point is that in "classical" atmospheres there is a unique correlation between temperature and depth, the same for all points on a star's disk. But it is not true for hydrodynamic models: now temperature distribution depends strongly not only on the depth, but on the points on the horizontal plane too.

It is clear that theoretical strengths of spectral lines for the case of homogeneous and inhomogeneous photospheres will be different, therefore the resulting abundances are different with $\Delta\log\varepsilon \approx \pm0.2 \div \pm0.3$ (by guess).

Depending on your point of view it will be fortunate or unfortunate that the assumption about uniform composition throughout the atmosphere may be wrong for some type of stars. Twenty years ago Michaud showed that the diffusion was the main course of building of abundance stratification in the atmosphere of chemical peculiar stars. But for a bulk of "ordinary" stars we hope that the assumption about uniform composition is still working.

LTE OR NON-LTE? HOT STARS

The most crucial question in the model atmosphere and line formation problem is the assumption of local thermodynamic equilibrium. About 60 years the astrophysicists at their symposiums or "coffee-breaks" could not avoid the discussion between LTE partisans and non-LTE partisans.

General approach in building the model atmospheres and in the determination the emergent spectrum is to find for each depth *d* the vector with many components:

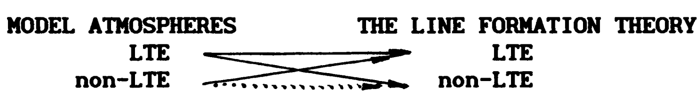
$$\begin{aligned}\psi_d = \psi_d\{&(J_1,J_2,\ldots,J_{NJ});N;N_e;T;(N_1(H),N_2(H),\ldots,N_{NLH}(H));\\ &(N_1(HeI),N_2(HeI),\ldots,N_{NLHEI}(HeI));\\ &(N_1(HeII),N_2(HeII),\ldots,N_{NLHEII}(HeII);N(HeIII);\\ &((N_1(El_i),N_2(El_i),\ldots,N_{NEl_i}(El_i)),i=1,NLEl);N_p\}\end{aligned}$$

Each component must be determined through the system of coupled equations:

1) the transfer equations specifying the mean intensity J for NJ number of frequencies;
2) the hydrostatic equilibrium equation specifying the total number of particles N;
3) the radiative equilibrium equation specifying the temperature T;
4) the equation of total particle conservation which specify N_e-electron density;
5) $(NLH+NLHEI+NLHEII+\Sigma NLEl_i)=NL$ rate equations for energy levels of atoms; they determine level populations;
6) the charge conservation requirement specifying the proton density N_p.

LTE assumption in the model atmosphere theory means that one avoids the resolve the equations (5) coupled with others. Full LTE assumption in the line formation theory (for the abundance determination) means that one is lazy to resolve the equations (1,5) only, because other equations have been already resolved in a fixed model atmosphere. In this case there is no need to perform any calculations (!). Thus the question "LTE or non-LTE?" is obviously not the question of a principle, but the question of our laziness.

There are several possibilities for the abundance determination. They are shown on the following scheme:



The most logical way is to follow the dotted arrow. This approach has been realized for hot stars only and for hydrogen-helium spectrum [38].

The latest achievements in the non-LTE building of model atmospheres must be connected with German team. Some NLTE models have been constructed by the well-known complete linearization method (CLM). But in some cases CLM fails [48]. Another method by Scharmer [49] has difficulties also. German group of theoreticians has developed a new method of approximate Λ-operators (MALO) which is becoming a standard technique for computations of NLTE models [50-51].

MALO considers the depth coupling accomplished by the radiative transfer only in the formal solution excepting the intrinsically contained core saturation approximation of Rybicki [52]. The time scale of computations is nearly the same as for CLM, but new refinements are allowed compared with CLM:

- increase the number NL of levels included;

- increase the number NT of line transitions included;
- increase the number NF of frequency points for numerical integrations of mean intensity J;
- refinement of line absorption coefficient (accounting for Voigt-Stark broadening).

In the CLM only a small numbers NT, NL and NF may be used: typically NL=9, NT=6, NF=65. Rauch and Werner [53] applying MALO were able to increase NL=15, NT=105. They have found that the change in NL and NT heats the outer layers substantially (fig.2).

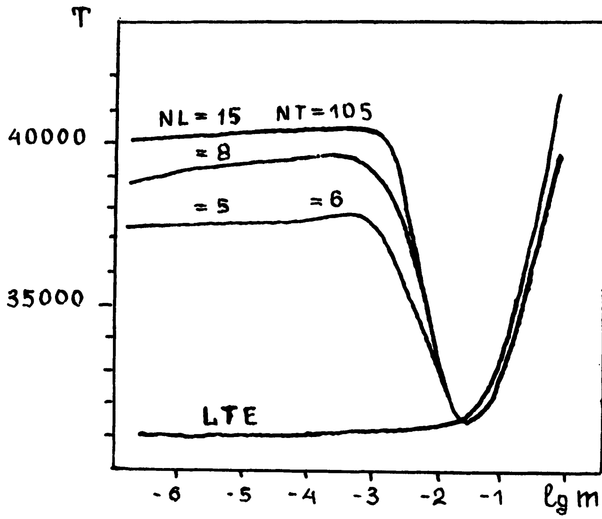


Figure 2. Temperature distribution of hydrogen model atmosphere at T_{eff} = 40000 K, log *g* = 4 for different NL and NT.

This heating becomes more pronounced when more and more levels and lines are included. Thus, model atmospheres with unsufficient values NL and NT are meaningless for upper layers. This conclusion is also true for medium temperature stars with T_{eff} = 9500 K + 15000 K [54].

Figure 2 allows to give such comment: LTE models always stayed cool in upper layers, Mihalas and Auer compelled models to be hotter, but German group found much hotter place.

For accurate model calculations we are to include the thermodynamic effect of *all* the atomic transitions (effect called usually "blanketing"). A few years ago the LTE constraints for atomic statistics could not be excluded for "blanketing" effect due to limited computer ability and the absence of special algorithms of NLTE computations with thousands lines.

Anderson [55] was the first who treated the NLTE blanketing effect. He developed a multy-frequency/multy-grey algorithm which admits the inclusion of hundreds lines arising from 30 levels. Figure 3 shows the temperature structure for the Anderson's model for three different cases.

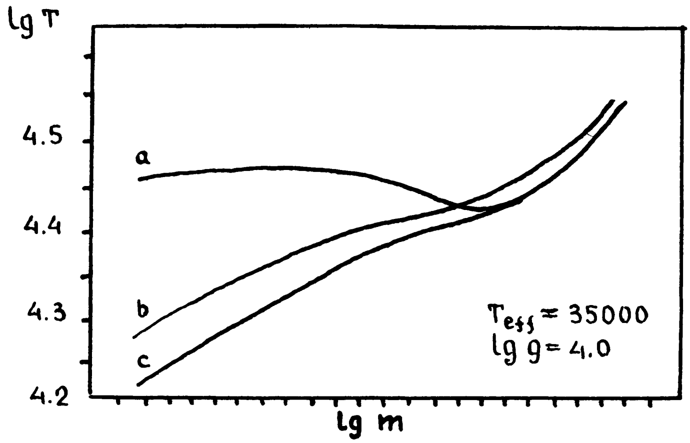


Figure 3. Temperature structure for: a) NLTE model by Mihalas; b) LTE model + LTE blanketing; c) NLTE model with NLTE blanketing.

The dramatic difference in the temperature structure between "classical" NLTE model by Mihalas and the new model by Anderson is clearly seen. A strong cooling of upper layers comes from the important role of the resonance lines CIII and CIV. And again the model constructing people found their cool place!

Can this loitering between hot and cool places change the abundance determination for hot stars?

Werner [56] computed the H-He profiles for two types of hot models (with and without NLTE blanketing) and found that profiles changed marginally because the lines were formed in much deeper layers where there were no large differences in the temperature structure. The same conclusion is true for the cooler model by Anderson as well. These results are very important because they give us a chance to assume that all previous hot models are quite reasonable for interpretation of lines in the visual part of spectrum.

Is this optimistic point of view true for lower temperature stars, say with T_{eff} < 25000 K? To answer this question we compared the results of the equivalent width calculations [41] based on different types of models: NLTE model with "chromospheric" rise in temperature in upper layers; quasi-NLTE model computed with SUM1-code; LTE model by Kurucz. It was found that the differences in W_λ for various models produce the error $\Delta \log \varepsilon$ of order $\pm 0.10 \div \pm 0.20$. This value is probably the limit in the accuracy of the abundance determinations for medium temperature stars. Present status of model atmospheres does not allow to obtain better accuracy.

Having discussed the uncertainties in the theory of model atmospheres, let me pay brief attention on the line formation theory for hot stars. Using the NLTE approach in the line formation one should resolve the coupled system of rate and transfer equations simultaneously. There are several computing codes for this procedure: LINEARA [57], LINEARB [58], TULIPE [59], MULTI [60], NONLTE3 [61]. The review of old NLTE computations is given in the book by Underhill and Doazan [62]. Among recent results I should mention the papers by Becker and Butler [63-64].Their results (table 2) give a strong prove of the necessity of the NLTE approach. One can see that LTE abundance may give systematic wrong results ($\Delta\log\varepsilon \approx -0.20$) compared to the NLTE values.

Table 2. LTE and NLTE abundances of N and O for two stars.

v_{turb}	lg ε(N) NLTE	lg ε(N) LTE	Δlg ε	lg ε(O) NLTE	lg ε(O) LTE	Δlg ε
	τ Sco	T_{eff} = 33000 K		lg g = 4.15		
0	-3.99	-3.80	-0.19	-3.16	-3.02	-0.14
5	-4.04	-3.87	-0.17	-3.30	-3.20	-0.10
10	-4.09	-3.95	-0.14	-3.42	-3.37	-0.05
	10 Lac	T_{eff} = 38000 K		lg g = 4.25		
0				-2.92	-2.91	-0.01
5				-2.97	-3.03	+0.06
10				-3.02	-3.15	+0.13

Let me demonstrate another important result. Due to complex interlocking between line transitions some lines may be filled by additional emission, so the LTE and NLTE line strengths differ substantially. In some cases even emission lines may be present in spectra of main sequence stars. This effect was found for NIII [65], CIII [61], NIV [66].To avoid the ambiguous results in the abundance determinations such lines must be excluded for abundance analysis. But to find such lines simply means to perform NLTE calculations!

The concluding remark of this section is following. The present status of the hot atmospheres theory permits to get the abundances with the accuracy not better than $\Delta\log\varepsilon = \pm0.10$. Additional steps should be undertaken to decrease this value. In other words the high S/N spectroscopists with record values $\Delta\log\varepsilon = \pm 0.05$ left theoreticians behind!

LTE OR NON-LTE ? COOL STARS

The analysis of chemical composition of cool stars by the full NLTE approach is less wide-spread. Only in last years a few attempts have been undertaken to calculate the appropriate NLTE model atmospheres. The most optimistic result comes from the paper by Ayres and Wiedemann [67].

They concluded that departures from LTE were small, even for low-density case of red giants. So LTE models are quite satisfactory for wide region of stars in the cool part of the H-R diagram, especially for F-K dwarfs and subgiants.

At the same time in extensive collaborative project Carlsson, Gratton, Gustafsson, Kiselman and Lemke perform radiative-equilibrium calculations for many elements without LTE assumption for F-stars and metal poor giants. They have shown that there are great departures from LTE. The final aim of this project is the building of self-consistent model atmospheres. This work is still in progress and it's result will clear up the problem of NLTE models for cool stars.

This uncertain status of cool stellar atmospheres modeling compels us to use LTE models with the LTE line formation theory (in *most cases*) and with departures from LTE (for few cases only).

In 1981-82 Duncan [68] and Spite & Spite [69] claimed that imperfections in modeling and the line formation theory including the LTE assumption lead to the abundance uncertainties $\Delta \log \varepsilon = \pm 0.05$. Their far-stretching statements were based on the abundances derived under the LTE approximation which they feel is justified in view of small NLTE effects Müller et al. [70] found in the Sun in 1975. Do recent results prove this conclusion or arguing in this way may be premature? Our reply to this question is *negative*!

Gigas [2] in his comprehensive study of Vega has shown that the NLTE corrections $\Delta \log \varepsilon = \log \varepsilon(\mathrm{NLTE}) - \log \varepsilon(\mathrm{LTE})$ for FeI vary between 0.26 and 0.44, the mean value $\Delta \log \varepsilon = 0.32$. For FeII lines these corrections are small: $\Delta \log \varepsilon = -0.02$. The same value for FeI ($\Delta \log \varepsilon = +0.30$) and for FeII ($\Delta \log \varepsilon = 0.00$) have been found by Lemke [1] for 16 sharp lines main sequence stars. At the same time for Vega small the NLTE corrections ($\Delta \log \varepsilon = -0.03$) are found for MgI-II weak lines [2], but strong lines give $\Delta \log \varepsilon = -0.10$. There are NLTE effects for Ba ($\Delta \log \varepsilon = +0.29$) [2].

Steenbock and Holweger [71] have solved the NLTE radiation transfer problem for LiI for different types of stars: the Sun, a K3 Ib supergiant, halo dwarf and halo giant. For the Sun and halo dwarf the NLTE effect has negligible influence on the derived Li abundance while for metal-rich and metal-poor supergiant the errors $\Delta \log \varepsilon = 0.30$. For the star 9 Boo Pavlenko [72] found $\Delta \log \varepsilon = 0.30$ also.

The next example comes from the paper by Magain [79] who showed that there were large NLTE effects in the abundance determination of different elements. Resulting corrections $\Delta \lg \varepsilon$ lie in the interval $0.18 \div 0.59$.

Our Kazan numerical NLTE experimentations have also proved the importance of NLTE effects. For solar-like subdwarfs we have confirmed well-known strong overionization for FeI. This leads to the systematic errors in the Fe abundance under the LTE assumption. Moreover this gives the uncertainties in the spectroscopic determination of lg g [73]. For barium the LTE corrections have values $\Delta \log \varepsilon = 0.12 \div 0.22$ [74]. Strong overionization of FeI takes place for yellow supergiants too [75]. At the same time for these stars sodium abundance is slightly influenced by NLTE effects ($\Delta \log \varepsilon = 0.02 \div 0.06$) [76]. Begley and Cotrell [77] found the systematic differences in the Na and Al abundances for disc dwarfs and giants. They ascribed these differences $\Delta\log\varepsilon \approx 0.3$ to the departures from LTE.

If we collect all values $\Delta\log\varepsilon$ mentioned in above cursory information, we shall see that $\Delta\log\varepsilon$ may lie in the interval $(-0.17) \div (+0.49)$ and even more. The worst is that: a) $\Delta\log\varepsilon$ may happen to be small or large for the same type of stars, but for different elements; b) $\Delta\log\varepsilon$ may happen to be small or large for the same element, but for different types of stars. No a priori estimation could be made! I should like to remind that the values $\Delta\log\varepsilon = (-0.17)\div(+0.49)$ are usually the subject of discussion among the stellar evolution and galactic chemical evolution people. Probably our symposium is not exception.

Three questions appear after this discussion. What can we conclude from the enormous number of the LTE determinations? Why are the spectroscopists so addicted to LTE? Why have we forgotten the main conclusion of rather old paper by Dumont et al. [78]: "We would appear to have shown that in order to obtain an abundance correct better than factor 3, it is necessary in each case to compute how important are the departures from LTE... Until a detailed non-LTE study is performed no such conclusion (about the reliability of the LTE abundance-N.S.) can be drawn a priori, either for any ion, or for any star".

Let me give an answer to all these questions according to personal philosophy. All LTE papers remind me a very ancient joke about Hodza Nasreddin who tried to find the lost money under a street lamp while he has lost them far away, in a dark place.

Finally I would like to adduce a rather long quotation from the paper by Magain [79] which reflects my personal point of view: "Although it might turn out that the classical LTE analysis are not always as bad as would appear from this paper, we have shown at least, that some non-LTE effects may be present in the atmospheres of Pop II stars, and may have important consequences as far as the relative abundances are concerned.The solution of this problem is in our opinion in our hand: we have instruments to investigate these effects and the theoreticians are beginning to have the appropriate non-LTE codes. It is just a matter of will: do we intend to continue to provide the galactic evolution theorists with data we cannot reasonably guarantee their reliability, or will we concentrate part of our efforts on checking the validity of our assumption?"

A few NLTE people who are not asleep or are not sitting back in this hall should applause to P.Magain for his claim for "perestroika" in our mind.

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