CHEMISTRY IN STELLAR ATMOSPHERES: THEORETICAL STUDIES AND COMPARISON WITH OBSERVATIONS

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ABSTRACT. The construction of model atmospheres is an eight-fold pathway. These pathways are described, with special reference to the chemistry of cool stars. A brief review of the present state of the art is presented, highlighting the outstanding problems. A few salient results are mentioned.

INTRODUCTION

We will confine this review to cool stars. These stars form a rather inhomogeneous group. The chemical composition may be different in different stars and masses are not known with certainty. To add to the confusion, most of the stars show variability - periodic and aperiodic. The extent of the atmosphere of some of the stars is so large that it may cover a substantial fracation of the radius, and mass loss is a way of life, especially in the case of Mira variables and supergiants. However, one thing is common - they are haven for molecular chemistry, and the particulate matter that one finds in the circumstellar shells and interstellar medium owes its nucleation to the atmospheres of these stars to a substantial extent. These aspects are challenging as well as awesome to the builder of atmospheric models. The progress has been slow but impressive gains have been made during the last two decades or so. Several articles have reviewed the past progress in the field (Vardya 1970, Johnson 1972, Wallerstein 1973, Carbon 1979) with Johnson (1986) bringing it upto date. Most of this progress has been, however, confined to giant and supergiant cool stars.

The construction of a model atmosphere is an eight-fold pathway as illustrated in Figure 1. The designation of each pathway is given in the core sectors, and the options available in each pathway are listed as we proceed outward. The simplest models are the ones based on the first options in each pathway. The models become progressively more sophisticated and realistic but difficult to compute as we choose higher options in one or more pathways. So far no models have been attempted with all the outermost options.

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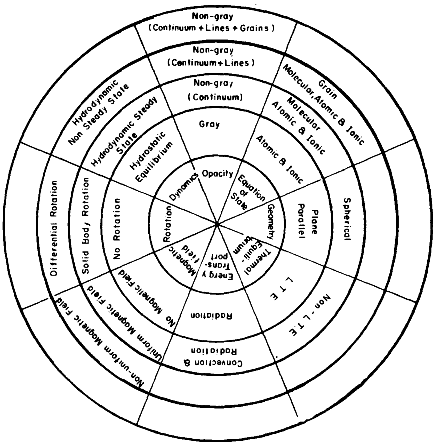

Fig. 1. Eight-fold pathway for construction of model atmosphere

EQUATION OF STATE

In solar composition cool stars, the main constituents of the equation of state are H_2,H,H^+, He and e; in peculiar composition stars, this may be different. However, for proper evaluation of electron pressure, and for opacity calculations, it is imperative to consider all important molecules formed out of the elements considered.

For n elements with a given relative elemental abundance, pressure, and temperature, one has to solve, in thermal equilibrium, n simultaneous equations. Equilibrium constants (K_p) used in these calculations are as good as the dissociation/ionization/detachment energies and the partition functions used. The partition functions for molecular negative ions except in a few cases, is assumed to be the same as that of the parent molecule. Spectroscopic constants for a few important negative ions like CN^- and C_2^- are not accurately known; note that $A^2\Pi u$-$X^2\Sigma^+$ lines of C_2^- may be observable in infrared spectra of carbon stars (Vardya and Krishna Swamy 1980), if and when accurate spectroscopic values of A state become available. We still do not know whether H_2^- is a stable ion or not. It may be worth including S_2^- not considered so far.

A close look at the updating of spectroscopic constants of diatomic molecules by Huber and Herzberg (1979) shows that dissociation energies and other constants for quite a few important molecules need to be improved or determined, like MgO, Tio, Zro and SiN; D_o^o (CN) has been given as 7.76 eV in the compilation but recent determination puts it at 7.95 eV (Colket 1984). Using the basic data from Huber and Herzberg (1979), Sauval and Tatum (1984) have given polynomial fits for partition functions and equilibrium constants for 300 diatomic molecules valid between 1000 - 9000^oK.

To understand the importance of different molecules at different stratification of a model atmosphere, one can plot march of molecules as a function of optical depth. This was attempted by Vardya (1966a) with about 100 species formed out of 15 elements, using a gray model atmoshere with sphericity, molecular band opacity and convection incorporated. Far refined plots can now be made using molecular equilibrium calculations, e.g. of Tsuji (1973) who considered 36 elements or Sauwal (1976) who considered 83 elements and 1600 compounds coupled with model atmospheres of Tsuji, or Johnson and his coworkers, or of Bell-Gustafsson collaboration (Johnson 1986).

The molecular abundances have been found to be very sensitive to the C/O elemental abundance ratio, or rather C-O difference, as CO is the most stable diatomic molecule (cf. Virgopia and Vardya 1971). In carbon stars, Si/S being greater or less than unity plays a similar role (Tsuji 1973); if $Si/S>1$, SiS, SiO, SiH, SiC_2 are the abundant molecules and if $Si/S<1$, SiS, CS, H_2S, HS and SiO dominate among the molecules of Si and S.

Condensation

Drastic temperature drop takes place, when sphericity is considered (Schmid-Burgk and Scholz 1981), in the outer layers of cool giant and supergiant stars. This may induce condensation in these layers. Many of these stars show signatures of grains in their circumstellar shells. It is very likely that nucleation may have taken place in the upper photosphere and these seed nuclei may have accreted matter in their outward journey. However, nothing can be said about the formation of grain in the photosphere as the theory of nucleation is still rather uncertain (cf. Draine 1981).

In M stars ($C/O<1$), grains, if formed, are perhaps of pure silicates whereas in C stars ($C/O>1$) of graphite or SiC (Mc Cabe 1982), with impurities picked up in their outward mass flow. If condensation does take place, depletion of certain species in gaseous form will occur and needs to be taken into account (cf. Alexander et al 1983).

Though a few computations have been attempted to incorporate grains in the construction of model atmospheres, it has been generally ignored due to lack of knowledge about the point of condensation.

SOURCES OF OPACITY

Vardya (1970) had given an extensive survey of sources of opacity in cool stars. Since then, a large effort has gone in computing line opacitiies for a large number of molecules, diatomic - CO, CN, C_2, CH, NH, OH, TiO, MgH, SiH and CaH, and polyatomic - H_2O, HCN and C_2H_2 (Alexander et al 1983, Tsuji 1976, Bell et al 1976). For some of these molecules, all the transitions have not been considered due to lack of basic data and for some others only crude oscillator strengths have been used. Line opacities due to SiO, SiS, CS, SiC, VO, ZrO, SiC_2, C_3 and C_2H, among others, may be important, but have not been computed. Not all the molecular opacities, enumerated above, have been incorporated by all the builders of model atmospheres. Some of the problems faced in including molecular line opacities are:
(i) Number of lines, due to vibration-rotation bands, besides electronic, are very large. Kurucz has recently considered 17 million atomic and molecular lines and still not considered all the molecules. Sharps

has considered 20 million lines for HCN (with various isotopes) only. Therefore, one has to consider mean (straight/harmonic), opacity distribution function, random sampling method or/and Voigt-Analog-Elsasser Band model to incorporate line opacities; all of these have advantages and disadvantages. (ii) Flux escapes through weak lines. Hence it is essential to consider a very large number of lines besides a few strong ones. (iii) Cool stars show a variety of elemental abundances and isotope ratios. Hence a few set of opacity tables (except the straight mean type) are not sufficient. (iv) It is assumed that the lines are formed in pure absorption. This need not be valid in tenuous atmospheres of cool giant and supergiant stars. (v) Turbulent velocity, an unknown parameter, goes into the computation of line opacity. (vi) In dwarf stars, pressure broadening is important, specially for rotational transitions, but is difficult to incorporate.

Let us pause and ask: "Is it worth considering these millions of lines, just because we have large computers, when finally we have to deal with a few "average quantities?" "Can one not evolve a simplified approach, having the same information content, as the one we end up with after reducing the millions of lines to a few hundred average values," using, say, the information theory?"

Grains

If grains exist in the photosphere, they will contribute significantly to the opacity (cf. Alexander et al 1983). These grains will not only play a role in the mass loss from these stars but may be related to the pulsation (Woodrow and Auman 1982) as well. Though the extinction due to grains can be calculated using Mie theory, the question of composition, size distribution and number density makes the whole exercise highly uncertain.

THERMAL EQUILIBRIUM

Most of the model atmospheres, computed so far, assume L.T.E. However, the facts that one sees lines of AlH due to 'inverse predissociation', 19 eV IR HeI triplet at λ10830Å and lines of other elements from high excited states (cf Chauville et al 1970), CaII H and K, MgII h and k, and FeII emission lines as well as intercombination lines in cool stars lead us to the conclusion that non-L.T.E. exists in these stars, specially in the outer layers, though some of these features may have chromospheric origin. Attempts have been made to examine the departures from L.T.E. in the population of H^- and in electron pressure (Kalkofen 1968, Auman and Woodrow 1975); significant effects are noted only at optical depths less than 0.1. Hence, it may hardly effect the temperature and pressure stratification of the atmosphere as well as the visual and infrared flux.

ENERGY TRANSPORT

The convective instability sets in at a rather shallow optical depths in cool stars, because of dissociation of molecular hydrogen and continues deeper due to hydrogen ionization. This does not ensure that convective mode of energy transport is efficient. In fact, an extensive superadiabatic zone exists, especially in the outer envelopes of giant and supergiant stars. Presently, there is no satisfactory theory to treat superadiabatic zone and the frequently used formalism (Böhm-Vitense 1958) or its variations (cf Deupree 1979) are at best a crude approximation with several arbitrary parameters (cf Henyey et al 1965).

A large number of model atmospheres have been constructed neglecting convection as it does not carry much flux. However, with better opacities, convection may be more efficient than found previously. Besides, it is not the turbulent pressure but its gradient which effect the pressure stratification. That is why, some of the models computed using constant turbulent velocity do not alter the structure significantly.

Most of the computations, in which convection has been incorporated, have ignored overshooting, which can change the structure and chemical composition of the atmosphere significantly.

If pulsation is present, one has to properly treat the dependence of convection on the pulsation phase (Deupree 1977).

Convection can also alter the molecular abundances from equilibrium values (cf Vardya 1972) if molecular relaxation time is longer than the convective time scale.

Note that the treatment of convection presents the greatest challenge in the construction of model atmospheres, and will remain a serious source of uncertainty till our understanding improves in this regard.

GEOMETRY

Plane parallel geometry is a reasonable assumption when the extent of the atmosphere, Δr, is very small relative to the radius, R, of the star. This holds well for cool dwarf stars, but for giant and supergiant stars, this need not be valid (cf Vardya 1982). In spherical symmetric atmospheres, specific intensity of radiation is a function not only of depth but of polar angle ($\cos^{-1}\mu$) as well; this complicates the calculations. Nevertheless, a few models for cool stars with spherical geometry have been computed and their ramifications examined (cf Watanabe and Kodaira 1978, 1979, Schmid-Burgk, Scholz and Wehrse 1981; Wehrse 1981; Scholz 1985). Far lower temperatures are reached in spherical atmospheres relative to comparable plane-parallel atmospheres, leading to significant changes in the abundance of molecules and formation of grains, besides the fact that contribution of scattering on the electronic molecular transitions may be substantial. It is not possible to predict the extension effects of these atmospheres, strongly controlled by molecular opacities, without detailed computations, as the molecular and grain formation depend sensitively on temperature (Schmid-Burgk, Scholz and Wehrse 1981). The structure and extension of these spherical models are also very sensitive to relative elemental abundances (Wehrse 1981).

In an extended atmosphere, the radius of the star is a frequency dependent quantity and may vary significantly (cf Bonneau and Labeyrie 1973). This fact may be used in constructing empirical model atmospheres, specially for cool supergiants (Vardya 1977).

FLUID DYNAMICS

The assumption of hydrostatic equilibrium is a very reasonable one in a homogeneous plane parallel atmosphere and has been the corner stone of a 'classical' atmosphere. However, in cool giant and supergiant stars, in which sphericity is almost a must, though not universally adopted due to computational difficulties, this assumption leads to some inconsistencies (cf Cassinelli 1971), as in the outermost layers, particles will be streaming outward with nearly radial velocity, with velocity distribution being not isotropic (Opik and Singer 1959). This implies that spherical geometry demands stellar wind. Outward mass motion can be in steady state or sporadic with or without shock waves. To make matters worse, this mass motion has to be coupled with the variability of most of these stars. This has not been done so far.

ROTATION AND MAGNETIC FIELD

Cool stars rotate very slowly. Therefore, rotation may not play any important role singly.

There are about half a dozen cool stars for which magnetic field has been established. Most of these measured fields are less than 2000G. They can influence appearance of molecular spectra, when observed at high dispersion (cf Schadee 1978).

The coupling of rotation and magnetic field with convection in the photosphere is the cause of stellar activity and has important consequences. We will not discuss it here as it will take us outside our purview.

ATMOSPHERIC MODELS

Johnson (1986) has summarized the range of models so far computed. There are three main groups, R.A. Bell and B. Gustafsson and their collaborators, H.R. Johnson and his associates, and T. Tsuji, who have been active in constructing cool star model atmospheres. Earlier, F. Querci and M. Querci had produced a large number of models for carbon stars. Most of these non-grey models are based on homogeneous plane parallel geometry, hydrostatic equilibrium and L.T.E., some have convection incorporated, others not; most of them have molecular line blanketing in some form or other but not grain opacity. Temperature range is 4200 to 2400°K and of log g 3 to -2; the coverage within these ranges is patchy. Besides solar elemental abundances, a few other compositions have also been tried.

Heidelberg group (J. Schmidt-Burgk, M. Scholz and R. Wehrse) has been mainly instrumental in pursuing the construction of model atmospheres for cool stars with spherical geometry. Scholz and Tsuji (1984) have computed spherical models appropriate for carbon stars.

As stated earlier, there are hardly any models pertaining to cool dwarf stars.

SOME SALIENT RESULTS AND COMPARISON WITH OBSERVATIONS

(i) When line blanketing (in pure absorption) is incorporated, the temperature in the outer layers is lowered, if the lines fall on the redward of flux maximum, as in the case of H_2O, CN, and CO, and is raised when the lines fall blueward of flux maximum, as in the case of TiO, NaI D, CaII H and K, and CaI 4227. Lowering of temperature in M supergiants may be $\sim 200^{o}K$ and in carbon stars $\sim 900^{o}K$. Surface temperatures may show further decrease when sphericity is considered and opacity due to polyatomic molecules or/and grains are included.

(ii) Atmospheric structures are rather different when computed using straight mean or harmonic mean line opacity. However, the column densities of various atomic or molecular species do not differ much in the two cases (Johnson et al 1975).

(iii) Comparison between observed and computed fluxes agrees reasonably except in the blue and at some of the molecular bands. UV excess in some of the models may be due to the neglect of some sources of opacity.

(iv) S stars have insignificant molecular opacity except for CO as C/O is very close to unity.

(v) Wherse (1981) found in spherical atmospheres that lowering the metal abundance increases the atmospheric extension and lowers the surface temperature in M supergiants. However, decrease in hydrogen abundance reduces the sphericity effect.

(vi) Carbon stars are less extended than comparable M stars (Scholz and Tsuji 1984).

(vii) Spherical models agree reasonably with observations of α Ori, o Cet and R Leo, and predict wavelength dependent radii (Scholz 1985).

(viii) Predictions based on models compare well (Piccirillo et al 1981) with semi-empirical relation between T_c and T_{eff} for K and M giants (Ridgway et al 1980). This temperature scale can also explain the colours of carbon stars (Tsuji 1981).

(ix) The molecular concentration of MgH has been used (Bell et al 1985) to determine the gravity of α Boo (K2IIIp). This can be extended to cooler stars as well.

(x) Bergeat et al (1976) find that for C Mira variables, $1500^{o}K \lesssim T_{eff} \lesssim 2300^{o}K$, excluding IRC+10216. Non-Miras have normally higher temperatures. Back warming effect due to grain and gas opacity may cause atmospheric oscillations (Woodrow and Auman 1982).

(xi) In C stars with $T_{eff} = 2500^{o}K$, the pressure in the model alters significantly when HCN is included as a source of opacity.

(xii) The predicted strength of H_2 quadrupole lines in C stars plane-parallel models (not spherical) with HCN and C_2H_2 opacity compares well with observations (Eriksson, et al 1984). Johnson et al (1985) find that H^- flux peak at λ 1.65μm disappears when hydrogen abundance is decreased; however, they have neglected HCN and C_2H_2 opacity and their models are also plane-parallel. Hence, it is difficult to say conclusively whether carbon stars are hydrogen deficient and helium enriched (Vardya 1966b).

(xiii) A large number of studies have investigated isotope ratios in cool stars, specially by Lambert and his associates, for red giants. Recently, Tsuji (1984) has computed elemental abundances and isotope ratios for α Her (M5 Ib-II), using a model atmosphere with $T_{eff} = 3250$, and $\log g = 0.0$, and Dominy et al (1986) have determined isotope ratios for four SC stars; most of these isotope ratios are far smaller than the solar system values.

CONCLUDING REMARKS

Improved values of partition functions, dissociation energies and transition probabilities are required for several important molecular species. The modus operandi of incorporating molecular line opacity needs a careful look; is there no satisfactory alternative to considering millions of lines? For supergiants and Mira variables, if not also for giant stars, spherical geometry with mass flow is a must. Last but not the least, any improvement in the treatment of convection will help greatly in improving the overall accuracy of cool atmospheric models and in understanding the chemistry in the atmospheres of cool stars.

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DISCUSSION

TATUM: When Kurucz performed his opacity calculations involving 17 million lines, did he treat each line individually, or did he generate them from the molecular constants?
VARDYA: I do not know the full details. Kurucz mentioned this fact as statistics at the IAU General Assembly Meeting at Delhi. He has considered a large number of atomic lines and for the diatomic molecules, he has included several isotopes also.

HUEBNER: (i) Regarding the question about Kurucz's line opacity, I believe that he used measured values whenever available and supplemented them with careful, theoretical calculations. (ii) In the past the practice was to use dust (grain) opacity from one source, molecular opacity from another source, and atomic opacity from still another source. These sources were inconsistent with each other in the equation of state and even in the basic atomic abundances. If I understand correctly, you now assume one consistent atomic abundance for the atomic, molecular, and condensed phases? (iii) Considerable progress has been made in the area of nucleation and condensation of carbon grains by Sedlmeyer and collaborators (Heidelberg - West Berlin group). Several of their papers have been published in the last 2 years in Astronomy and Astrophysics. Would this help to improve your condensation model? (iv) Many of the 20 million lines that you mentioned that Sharp (Los Alamos) has calculated are for isotopes of HCN only. These isotopic lines contribute only about 10% to the opacity if there is a small line broadening mechanism such as Doppler broadening from turbulence. Although it may be necessary to calculate individual lines for diatomic and linear triatomic molecules, isotope effects can be neglected in most cases and for non-linear polyatomic molecules, lines can be smeared, e.g., with the "just overlapping line model". Do you have any comments on this? (v) The (Rosseland) opacity is sensitive to the absorption coefficient between the absorption lines. Have you taken into account the continuum absorption from photodissociation and ionization of molecules?
VARDYA: Regarding your point (ii), I myself have not computed these opacities. This should be done, in a consistent way, as you have mentioned, and some attempts have been made in this direction. On (iv) I have no special comments. Regarding point (v), opacity due to photoionization and photodissociation has not been considered so far in computation of cool model atmosphere. A few years back, however, Tarafdar and his associates did incorporate OH continuum opacity in solar model.

SOMERVILLE: On the problem of dealing with very large numbers of spectral lines, I'd like to draw attention to a method of Statistical Spectroscopy introduced some years ago by C.W. Allen (M.N. 133, 21, 1966; 139, 367, 1968; 148, 435, 1970; also 168, 121, 1974 (Editors)) and developed in the thesis work of Jon Darius. It gives a good, systematic approach to the problem and works very well.

VARDYA: It will be interesting to look into it and compare with other methods currently in use.