Asymptotic Giant Branch Stars
T. Le Bertre, A. Lèbre and C. Waelkens, eds.
I.A.U. Symposium 191, 1999

Dynamical Modelling of AGB Star Atmospheres

Susanne Höfner
Niels Bohr Institute, Astronomical Observatory
Juliane Maries Vej 30, DK-2100 Copenhagen, Denmark

Abstract. Time-dependent dynamics is an important ingredient for understanding the atmospheres of pulsating AGB stars. The shock waves created by stellar pulsation modify the atmospheric structure and, consequently, influence the mass loss and the observable properties. So far, hydrostatic model atmospheres have been used in most cases to analyse photospheric spectra, neglecting the effects of dynamics. The recent progress in observational techniques, however, has demonstrated the importance of consistent time-dependent models. The main topics of this contribution are to discuss fundamental physical processes and technical problems in constructing dynamical model atmospheres, to review the present status of modelling and to indicate possible future developments.

1. Introduction

The atmospheres of AGB stars are strongly affected by time-dependent dynamical phenomena. Stellar pulsation creates shock waves which propagate through the atmosphere, changing its structure both on a local and a global scale (see Fig. 1). In the inner parts of the atmosphere the passing shocks cause a more or less periodic modulation of the structure. In the upper layers the dissipation of mechanical energy leads to a levitation, i.e. a density enhancement of up to several orders of magnitude compared to a hydrostatic atmosphere. Both of these effects influence the formation of molecules and dust grains and, consequently, the optical properties as well as the mass loss of these stars.

Up to now hydrostatic model atmospheres have been used in most cases to interpret observed photospheric spectra of AGB stars, neglecting the effects of dynamics on the atmospheric structure. While impressive results have been obtained with this approach for non- or weakly pulsating late-type stars, systematic discrepancies or misinterpretation may result in situations where dynamics plays a decisive role (see reviews by Gustafsson & Jørgensen 1994, Gustafsson 1998 and Plez, this volume).

On the other hand, for the last two decades dynamical models have been used to study mass loss by stellar winds and (more recently) optical properties of circumstellar dust shells, but mainly concentrating on objects with high mass loss rates and more or less optically thick dust envelopes (see Fleischer et al. and Winters et al., this volume). Due to computational reasons time-dependent dynamical models are generally based on a simple (grey) treatment of radiative transfer, in contrast to their hydrostatic counterparts. This approach works

https://doi.org/10.1017/S0074180900203021 Published online by Cambridge University Press

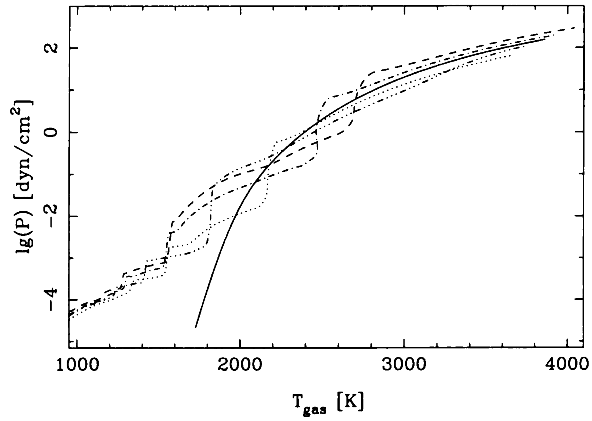

Figure 1. Influence of dynamics on the atmospheric structure (gas pressure vs. temperature): a dynamic model at different phases (0.50: dashed; 0.75: dash-dotted; 1.00: dotted; 1.25: dash-triple-dot) and the corresponding hydrostatic initial model (full line); phase 0.5 corresponds to minimum light, 1.0 to maximum light. The 'steps' in the pressure indicate shock waves. Their propagation through the atmosphere can be seen by tracking the progress of individual features from higher pressures and temperatures to lower ones (i.e. from right to left) with increasing time (phase 0.5 to 1.25). The periodic modulation of the inner parts of the atmosphere and the levitation of the outer layers are visible in this plot (model P7C14U4 of Höfner et al. 1998).

reasonably well if dust is the main opacity source but it is problematic when molecular features dominate (line blanketing).

The construction of realistic time-dependent dynamic models of the inner dust-free atmospheric layers which allow a quantitative prediction of observable properties for stars with optically thin circumstellar envelopes has to be considered as an open problem. However, in the last few years some progress has been achieved in this field and at least at a qualitative level the theoretical results are comparable with observations. Currently, several projects are devoted to improve the treatment of relevant physical processes.

2. Modelling methods: general concepts

In addition to the theoretical aim of understanding the atmospheres of AGB stars in terms of fundamental physics, the impressive progress of observational techniques achieved during the last few years requires a similar improvement of models. The simple picture of a (quasi-) static atmosphere surrounded by a stationary outflow is not adequate for a reliable interpretation of observational data with high spectral resolution (individual molecular bands originating in different atmospheric layers; line profile variations due to velocity fields), a wide wavelength coverage (simultaneous monitoring of molecular and dust features), high angular resolution (spatial structure of the atmosphere) and detailed monitor-

https://doi.org/10.1017/S0074180900203021 Published online by Cambridge University Press

ing of temporal variations of individual stars. This purpose requires consistent, time-dependent models which cover both the inner atmosphere and the stellar wind as well as the highly complicated transition region, taking the relevant physical processes into account.

Ideally, such models should be based on a self-consistent simultaneous solution of time-dependent dynamics (including a realistic treatment of stellar pulsation, shock waves and mass loss by a stellar wind), a detailed frequency-dependent radiative transfer (molecules, dust) and a full non-equilibrium treatment of micro-physical processes (chemistry, dust formation). However, present dynamic models are far from this ideal due to computational limitations and a lack of fundamental physical data. Even when using the assumptions of micro-physical equilibrium and LTE (with the possible exception of dust formation or thermal relaxation behind shocks) the remaining system of time-dependent dynamics and detailed frequency-dependent radiative transfer is far beyond the capacities of present-day computers. Therefore, in general a two-step approach is used to model atmospheres of long-period variables.

First, the variable structure of the atmosphere and circumstellar envelope is obtained by solving the equations of hydrodynamics together with a simple grey treatment of radiative transfer and a (consistent, time-dependent or parameterized) description of dust formation. At this stage, the pulsation of the star is simulated by a more or less sophisticated variable inner boundary which is located below the photosphere and accounts for the motions and luminosity variations induced by the pulsation. The immediate results of these dynamical calculations are mass loss rates, outflow velocities and dust-to-gas ratios. A comparison of the input physics and the results of present dynamical models produced by different groups can be found in the review by Woitke (1998). A short summary of results is given in Sect. 3.

In a second step, a detailed radiative transfer calculation based on the structures obtained in the dynamical computation yields the required observable properties: synthetic spectra at various resolutions and their variation with phase, photometric colours and light curves, spatial intensity distributions or line profile variations. An overview of these results is presented in Sect. 4. (see also Table 1).

3. Atmospheric structure and stellar wind

The pioneering dynamical calculations of Wood (1979) and Bowen (1988) demonstrated that the typical mass loss rates and wind velocities of LPVs are most probably due to the combined effects of stellar pulsation (shock waves) and radiative driving (dust). Furthermore, in both papers the considerable influence of thermal relaxation behind shocks (finite rate or immediate cooling) on the atmospheric structure and on the mass loss rate were discussed. The question of cooling rates (and the relevance of non-LTE processes in this context) is still a matter of debate (e.g. Woitke et al. 1996, 1998; Willson & Bowen 1998).

Fleischer et al. (1992) presented models for C-rich LPVs which include a consistent, time-dependent description of the dust formation process, demonstrating that the interaction of dynamics and dust formation can result in a shell-like structure of the circumstellar envelope. The strong coupling between

https://doi.org/10.1017/S0074180900203021 Published online by Cambridge University Press

Table 1. Papers on synthetic observable properties and references for the corresponding dynamic models (modelling methods).

dynamic models	observable properties	
Wood (1979)	Bessell et al. (1989) Scholz & Takeda (1987)	spectra, colours, radii (M) limb darkening, radii (M)
Wood (1990)	Bessell et al. (1996) Scholz (1992)	spectra, radii, line profiles (M) line profiles (M)
Bowen (1988)	Beach et al. (1988) Luttermoser & Bowen (1990)	limb darkening, radii atomic lines (non-LTE)
Fleischer et al. (1992)	Winters et al. (1994) Winters et al. (1995) Winters et al. (1997) Gauger et al. (1998)	light curves (dust) brightness profiles (dust) model for AFGL 3068 CO line profile variations
Höfner & Dorfi (1997)	Windsteig et al. (1997) Windsteig et al. (1998)	mid-/far-IR colours (dust) CO line profile variations
Höfner et al. (1998)	Loidl et al. (1997, 1998, 1999) Aringer et al. (1997, 1999) Hron et al. (1997, 1998) Alvarez & Plez (1998)	molecular spectra (C) molecular spectra (M) ISO-SWS spectra (C) colour variations (M)

thermodynamics, dust formation and dynamics may lead to instabilities (dust-induced κ-mechanism; Fleischer et al. 1995, Höfner et al. 1995) and to multi- or non-periodicity in the behaviour of the circumstellar envelope (e.g. Winters et al. 1994, Höfner & Dorfi 1997) since the dust component is governed by its own time-scales. First results of similar dynamic models for O-rich stars have been presented by Jeong et al. (this volume). For a review of dynamical wind models see Fleischer et al. (this volume).

Recently we have calculated a new set of dynamic models (Höfner et al. 1998) for the purpose of studying the time-dependent behaviour of IR molecular features. Instead of using a constant value to represent the gas opacity as in many earlier models (e.g. Bowen 1988, Fleischer et al. 1992, Höfner & Dorfi 1997) these new model atmospheres are based on Planck mean opacities computed from detailed frequency-dependent molecular absorption coefficients (SCAN data base, Jørgensen 1997). This has a considerable influence on the atmospheric background structure and consequently on the mass loss and observable properties.

Fig. 2 shows the pressure-temperature structures of several hydrostatic models with identical stellar parameters but using different treatments of the gas opacity and radiative transfer: the grey hydrostatic initial model[1] based on

[1] Our dynamical calculations start from models representing the hydrostatic limit case of radiation hydrodynamics. These initial models are defined by the following parameters: luminosity $L_\star$, stellar mass $M_\star$, effective temperature $T_\star$ and the carbon-to-oxygen ratio $\varepsilon_C/\varepsilon_O$

https://doi.org/10.1017/S0074180900203021 Published online by Cambridge University Press

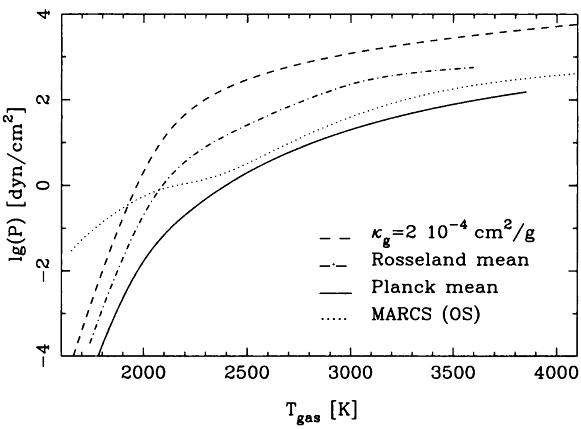

Figure 2. Influence of the radiative transfer and gas opacities on the atmospheric structure (gas pressure vs. temperature) of hydrostatic models: grey initial models based on Planck mean (full line) and Rosseland mean (dash-dotted) molecular absorption coefficients and on a constant value of the gas opacity (dashed) as well as a MARCS model atmosphere (dotted) based on full monochromatic opacity sampling of the same molecular data as in the mean opacity models. All models have the same stellar parameters ($L_\star = 7\,000\,L_\odot$, $M_\star = 1\,M_\odot$, $T_\star = 2\,880\,\mathrm{K}$, $\varepsilon_C/\varepsilon_O = 1.4$).

Planck means (full line) is in reasonable agreement with a MARCS model (dotted) which includes a frequency-dependent solution of radiative transfer, based on the same data for molecular absorption coefficients. In contrast, the model calculated with a constant gas absorption coefficient introduced by Bowen (1988) and used in many dynamic models (dashed line) shows a much higher density at a given temperature, leading to unrealistically strong molecular features. For comparison, a model based on Rosseland means of the same molecular data as used in the Planck mean and MARCS models is shown in Fig. 2 (dash-dotted). While the Rosseland mean is the correct mean to apply in the stellar interior (diffusion limit) it tends to underestimate the opacity in the atmosphere and leads to much higher densities than the Planck mean model.

The density differences in the hydrostatic initial models caused by different gas opacities are also reflected in the resulting wind properties of the dynamical models. The Planck mean models presented in Höfner et al. (1998) show reduced dust condensation and significantly smaller mass loss rates than those of Höfner & Dorfi (1997; constant gas opacity). Furthermore, the molecular opacities may contribute to driving the stellar wind. Fig. 3 shows an O-rich model calculated without dust formation which exhibits an outflow driven by radiation pressure on molecules with a typical wind velocity (12 km/s) and a mass loss rate of $\approx 10^{-6} M_\odot/\mathrm{yr}$. Note in this context that the driving by molecules only becomes efficient in the dynamical model where the radiation pressure acts on material which has already been lifted to cooler layers by the pulsation-induced

https://doi.org/10.1017/S0074180900203021 Published online by Cambridge University Press

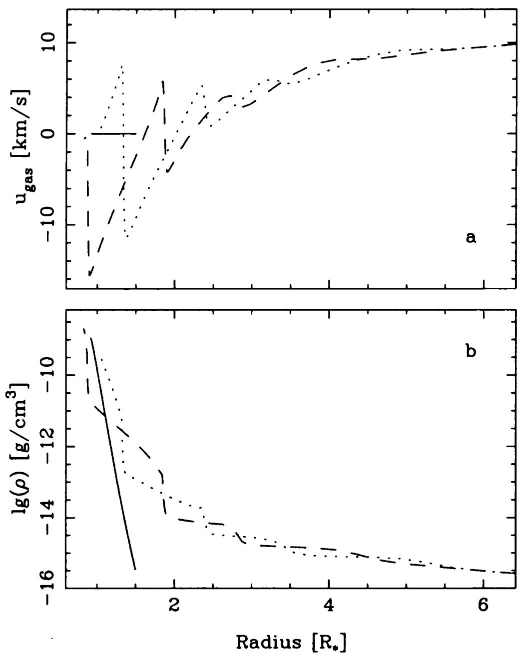

Figure 3. Radial structure of a dynamic model at different phases (0.50: dashed, minimum light; 1.00: dotted, maximum light) and of the corresponding hydrostatic initial model (full line); flow velocity (a) and gas density (b) as a function of the radius (given in units of the radius of the hydrostatic initial model). The wind of this O-rich model is driven by radiation pressure on molecules (no dust formation included). Model P7OU4 of Höfner et al. (1998).

shock waves. The corresponding non-pulsating initial model (full line) shows no tendency to form a radiation-driven wind.

Helling et al. (poster contribution, this conference) have investigated the influence of molecular opacities on stellar winds using Planck and Rosseland means to estimate upper and lower limits of the effects. The results for Planck mean models are in qualitative agreement with Höfner et al. (1998) while models based on Rosseland mean opacities largely resemble earlier models based on a small constant value of the gas absorption coefficient (e.g. Fleischer et al. 1992, Höfner & Dorfi 1997).

4. Observable properties of dynamic models

Regarding predictions of observable features, the existing dynamic models can be divided roughly into two groups: models for dust-enshrouded stars hidden in their circumstellar envelopes (IR carbon stars, OH/IR stars) on the one hand and models for stars with optically thin (or non-existent) circumstellar envelopes ('optical' AGB stars) on the other hand.

For the first group the observable properties are determined mostly by outflow characteristics (mass loss rate, velocity field, spatial structure of the circumstellar envelope) and by the properties of the dust grains (chemical composition, grain sizes). Typical examples of predicted quantities are spectral energy distributions and spatial brightness profiles of the circumstellar envelopes, dust features, IR photometric colours and light curves, as well as line profile variations due to velocity fields (e.g. Winters et al. 1994, 1995, 1997; Windsteig et al. 1997, 1998; Gauger et al. 1998). For a more detailed discussion see the contribution of Winters et al. (this volume).

In contrast, stars with circumstellar envelopes that are more or less optically thin at NIR wavelengths can give valuable insights into the complex interactions of the time-dependent atmospheric dynamics with the formation of molecules and dust grains. Molecular features allow us to probe the critical transition region between the photospheric layers and the circumstellar dust shell where the mass loss is initiated.

Predictions of observable properties for stars with optically thin envelopes (e.g. molecular spectra) require a realistic treatment of the physics that governs the atmospheric background structure and the shock waves (e.g. gas opacities and radiative transfer, see Sect. 3.). A detailed *quantitative* interpretation of observational data is beyond the scope of present time-dependent models because they are based on some more or less crude physical assumptions (e.g. grey radiative transfer, piston boundary) due to computational restrictions. However, they give us some *qualitative* understanding of intrinsically time-dependent phenomena which are not accessible with hydrostatic models.

Early exploratory studies of the effects of atmospheric extension on observable properties of M-type Mira stars were performed by Bessell et al. (1989) and Scholz & Takeda (1987). Using parameterized density structures similar to the models of Wood (1979) they obtained IR spectra and a phase and wavelength dependence of monochromatic radii in reasonable agreement with observations.

Limb darkening for extended atmospheres with shocks and the effects on angular diameter determinations by lunar occultation observations were studied by Beach et al. (1988) using the dynamic models of Bowen (1988) and simple radiative transfer. Luttermoser & Bowen (1990) discussed first results of non-LTE radiative transfer calculations for atomic lines.

Based on the pulsation models of Wood (1990), Bessell et al. (1996) investigated the photospheric structure and observable properties of Mira variables. The general appearance and the variability of the resulting synthetic spectra which were used to derive monochromatic radii are in good agreement with observations. The velocity fields lead to a complex time-dependent behaviour of absorption line profiles and influence the integrated line strengths (Scholz 1992). Certain features do not only show a variation with phase but also differ at a given phase from cycle to cycle, reflecting a non-periodic behaviour of the atmospheric layers where they originate.

Recently, several studies of observable properties based on the dynamic model atmospheres of Höfner et al. (1998) have been presented. Alvarez & Plez (1998) used a dynamic model to explain phase shifts between different observed narrow band colours of M-type Mira stars (modulation of the structure by propagating shocks) which could not be reproduced with hydrostatic model

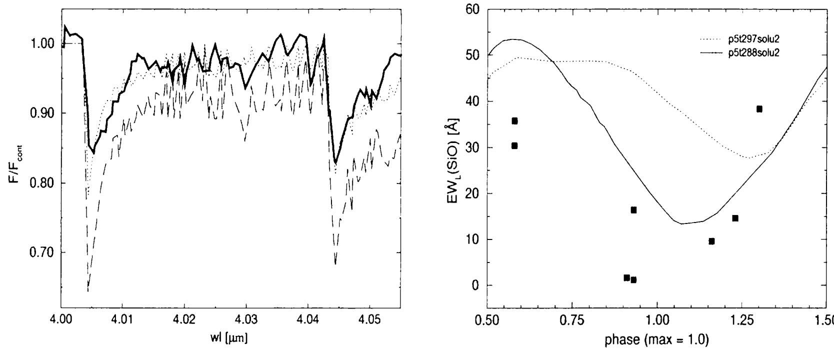

Figure 4. Theoretical and observed properties of SiO rotation-vibration bands: Left panel: a comparison of normalized spectra in the 4 μm region; observed spectrum of S Gru (full line) and synthetic spectra based on a dynamical model (dotted) and a hydrostatic atmosphere (dashed). Right panel: the corresponding equivalent width of the SiO bands as a function of the bolometric phase for two dynamical atmospheres (full and dotted lines) and as a function of visual phase for observed Mira stars (squares). From Aringer et al. (1999).

atmospheres. IR molecular spectra of carbon stars have been calculated by Loidl et al. (1997, 1998, 1999) and were compared to ISO-SWS observations by Hron et al. (1997, 1998 and this volume), demonstrating the potential of analyzing the stellar spectra and their variability with dynamic models. A confrontation of synthetic spectra of O-rich models (Aringer et al. 1997) with ISO-SWS data is presented in Hron et al. (1997) and Aringer et al. (this volume). At a higher resolution, the behaviour of SiO rotation-vibration bands around 4 μm has been studied by Aringer et al. (1999). While hydrostatic model atmospheres predict too strong features for very cool and extended objects, the experimental dynamic models are in principle able to explain the whole observed range of equivalent widths and their variations (see Fig. 4). Further constraints on atmospheric structure and velocity fields can be expected from a comparison of line profile variations of molecular lines with observations.

5. Recent developments and unsolved problems

Time-dependent dynamics is essential for understanding the atmospheres of pulsating AGB stars: it influences the structure both on global (levitation, wind) and local (shock waves) scales. Therefore, dynamic models are the only consistent way of studying temporal variations of observable properties. Existing dynamic model atmospheres give valuable insights into time-dependent phenomena and are in reasonable qualitative agreement with observations (Sect. 4.). However, due to a lack of computing capacities and of fundamental physical data they suffer from restrictions and approximations. Step-by-step improvements are necessary for a detailed quantitative understanding of observations.

https://doi.org/10.1017/S0074180900203021 Published online by Cambridge University Press

A more realistic (i.e. non-grey) description of radiative transfer seems to be one of the most pressing problems due to the considerable effect on the atmospheric background structure (see Sect. 3.). While a detailed treatment with thousands of frequency points as in hydrostatic models is far beyond the capacities of present computers, it should be possible to include frequency-dependent radiative transfer with a very limited number of frequencies in the near future. By systematically reducing the number of opacity sampling points in hydrostatic models Helling & Jørgensen (1998) demonstrated that as few as 50 frequencies may be sufficient to obtain better results than with mean opacities.

Another important point is the treatment of stellar pulsation. In most state-of-the-art dynamic models the pulsation is simulated by a variable boundary (piston) which is located beneath the stellar photosphere and moving sinusoidally with given velocity amplitude and period. In contrast, Bessell et al. (1996) and Scholz (1992) based their investigations on photospheric models calculated with a variable inner boundary derived from the dynamic models of Wood (1990). These models include the driving zone of the pulsation but introduce a depth-dependent free parameter (artificial damping/growth factor) into the energy conservation equation which is adjusted to produce the desired non-linear pulsation amplitude. Despite these problems of modelling the pulsation itself this is an interesting approach to define a more consistent boundary condition for the atmospheric calculation.

Regarding the impressive progress achieved in non-linear pulsation models for other types of variable stars during the last few years (e.g. RR Lyrae double mode pulsations, Feuchtinger 1998) fundamental improvements for LPVs can be expected in the near future. This would be an important step towards the long-standing goal of a simultaneous, self-consistent modelling of pulsation, atmosphere and stellar wind of AGB stars.

Acknowledgments. I thank U.G. Jørgensen, R. Loidl, B. Aringer (who also provided the plots shown in Fig. 4), J. Hron, E.A. Dorfi and M. Feuchtinger for inspiring discussions and helpful comments. This work was supported by the Austrian Science Fund (FWF; grants J01283-AST, J1487-PHY and S7305-AST).

References

Alvarez R., Plez B., 1998, A&A 330, 1109

Aringer B., Kerschbaum F., Jørgensen U.G., et al., 1997, in First ISO Workshop on Analytical Spectroscopy, ESA SP-419, p. 249

Aringer B., Höfner S., Wiedemann G., et al., 1999, A&A, in press

Beach T.E., Willson L.A., Bowen G.H., 1988, ApJ 329, 241

Bessell M.S., Brett J.M., Scholz M., Wood P.R., 1989, A&A 213, 209

Bessell M.S., Scholz M., Wood P.R., 1996, A&A 307, 481

Bowen G.H., 1988, ApJ 329, 299

Feuchtinger M.U., 1998, A&A 337, L29

Fleischer A.J., Gauger A., Sedlmayr E., 1992, A&A 266, 321

Fleischer A.J., Gauger A., Sedlmayr E., 1995, A&A 297, 543

https://doi.org/10.1017/S0074180900203021 Published online by Cambridge University Press

Gauger A., Winters J.M., Fleischer A., Keady J.J., 1998, in Cyclical Variability in Stellar Winds, L. Kaper and A.W. Fullerton (eds.), ESO Astrophysics Symposia, Springer, p. 309

Gustafsson B., 1998, Ap&SS 255, 241

Gustafsson B., Jørgensen U.G., 1994, A&AR 6, 19

Helling C., Jørgensen U.G., 1998, A&A 337, 477

Höfner S., Dorfi E.A., 1997, A&A 319, 648

Höfner S., Feuchtinger M., Dorfi E.A., 1995, A&A 297, 815

Höfner S., Jørgensen U.G., Loidl R., Aringer B., 1998, A&A 340, 497

Hron J., Aringer B., Loidl R., et al., 1997, in First ISO Workshop on Analytical Spectroscopy, ESA SP-419, p. 213

Hron J., Loidl R., Höfner S., Jørgensen U.G., Aringer B., Kerschbaum F., 1998, A&A 335, L69

Jørgensen U.G., 1997, in Molecules in Astrophysics: Probes and Processes, E.F. van Dishoeck (ed.), IAU Symp. 178, Kluwer, p. 441.

Loidl R., Hron J., Höfner S., et al., 1997, Ap&SS 251, 243

Loidl R., Hron J., Aringer B., Höfner S., Jørgensen U.G., 1998, Ap&SS 255, 289

Loidl R., Höfner S., Jørgensen U.G., Aringer B., 1999, A&A, in press

Luttermoser D.G., Bowen G.H., 1990, in Cool Stars, Stellar Systems, and the Sun, Sixth Cambridge Workshop, G. Wallerstein (ed.), A.S.P. Conf. Ser. 9, p. 491

Scholz M., 1992, A&A 253, 203

Scholz M., Takeda Y., 1987, A&A 186, 200

Willson L.A., Bowen G.H., 1998, in Cyclical Variability in Stellar Winds, L. Kaper and A.W. Fullerton (eds.), ESO Astrophysics Symposia, Springer, p. 294

Windsteig W., Dorfi E.A., Höfner S., Hron J., Kerschbaum F., 1997, A&A 324, 617

Windsteig W., Höfner S., Aringer B., Dorfi E.A., 1998, in Cyclical Variability in Stellar Winds, L. Kaper and A.W. Fullerton (eds.), ESO Astrophysics Symposia, Springer, p. 308

Winters J.M., Fleischer A.J., Gauger A., Sedlmayr E., 1994, A&A 290, 623

Winters J.M., Fleischer A.J., Gauger A., Sedlmayr E., 1995, A&A 302, 483

Winters J.M., Fleischer A.J., Le Bertre T., Sedlmayr E., 1997, A&A 326, 305

Woitke P., Krüger D., Sedlmayr E., 1996, A&A 311, 927

Woitke P., 1998, in Cyclical Variability in Stellar Winds, L. Kaper and A.W. Fullerton (eds.), ESO Astrophysics Symposia, Springer, p. 278

Wood P.R., 1979, ApJ 227, 220

Wood P.R., 1990, in From Miras to Planetary Nebulae: Which Path for Stellar Evolution?, M.O. Mennessier and A. Omont (eds.), Editions Frontières, Gif-sur-Yvette, p. 67