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Dynamical Atmospheres and Winds of AGB stars

S. Höfner and C. Sandin

Dept. of Astronomy & Space Physics, Uppsala University, Sweden

B. Aringer, A. C. Andersen and U.G. Jørgensen

Niels Bohr Institute, Astronomical Observatory, Copenhagen, Denmark

R. Gautschy–Loidl, W. Nowotny and J. Hron

Inst. f. Astronomy, University of Vienna, Austria

Abstract. We summarize the current status of our latest generation of model atmospheres for pulsating asymptotic giant branch stars, discussing effects of non-grey radiative transfer, dust grain properties and drift between gas and dust on the atmospheric structures and wind characteristics. In addition, we give an overview of the resulting synthetic spectra and how they compare with observations.

1. Introduction

Atmospheres of pulsating asymptotic giant branch stars are close to the 'worst case scenario' for realistic, self-consistent modelling: Propagating shock waves caused by stellar pulsation modify the structures of the atmospheres on local and global scales, causing strong deviations from hydrostatic stratification. The radiative fields are dominated by molecular opacities or even by dust grains forming in the cool outer layers of the atmospheres. Important micro-physical processes like gas-phase chemistry and dust formation may be severely out of equilibrium (see review by Woitke, this volume).

Even if we assume that the relevant physical and chemical input data exists, it is not feasible at present to model the coupled system of time-dependent hydrodynamics, non-LTE radiative transfer and chemical non-equilibrium, given the performance of existing computers. Therefore it is important to identify the most relevant processes in order to create models which are sufficiently realistic to allow a reliable interpretation of current observations.

At present, two types of models exist side by side. Classical hydrostatic model atmospheres include a sophisticated treatment of micro-physical processes and radiative transfer but neglect the effects of dynamics (pulsation, winds). On the other hand, time-dependent dynamical models for stellar winds tend to be based on crude descriptions of radiative transfer and simplified micro-physics, leading to unrealistic atmospheric background structures. Our recently developed model atmospheres which couple time-dependent dynamics and frequency-dependent radiative transfer (Höfner et al. 2002a,b) try to bridge the gap between these two types of models.

2. Dynamical model atmospheres

The modelling of the dynamical atmospheres is done in two steps: first, we perform a radiation-hydrodynamical calculation which gives the structure of the atmosphere and wind as a function of time, as well as a time-averaged mass loss rate, wind velocity and dust-to-gas ratio for a given set of stellar parameters. In a second step, we select snapshots of the structures as input for a detailed radiative transfer code to calculate synthetic observable properties which can be compared to observations (see Sect. 3.).

2.1. Modelling method

In this section we briefly summarize the main features of our dynamical models. For a more detailed description of the modelling method see Höfner et al. (2002b).

The variable structure of the atmosphere is obtained by solving the equations of hydrodynamics together with the frequency-integrated zeroth and first moment equations of the radiative transfer equation which describe the momentum and energy balance of the radiation field. The frequency-integrated opacities and the Eddington factor which are required to close the system of conservation equations result from a solution of the frequency-dependent radiative transfer equation for the given density-temperature structure at each time step. The models presented here are based on opacity sampling data of molecular opacities at about 50 randomly chosen frequency points.

The C-rich models include a time-dependent description of dust grain growth and evaporation, using the so–called moment method (Gail & Sedlmayr 1988, Gauger et al. 1990). The equations which determine the evolution of the dust component are solved simultaneously with the radiation-hydrodynamics system, assuming spherical grains consisting of amorphous carbon. At present, our models contain no description of grain formation for an O-rich chemistry. Therefore, when studying M stars we currently either assume that no dust is formed, or use a simple parameterized description of the dust opacity like Bowen (1988).

The dynamical computation starts with a dust-free hydrostatic initial model which is characterized by the following parameters: luminosity L_*, effective temperature T_*, mass M_* and the elemental abundances. The stellar pulsation is simulated by applying a variable inner boundary $R_{\rm in}(t)$ below the photosphere which is moving sinusoidally with a velocity amplitude Δu_p and a period P. Since the total radiative flux is kept constant there the luminosity at the inner boundary varies proportional to $R_{\rm in}^2$.

2.2. Atmospheric structures and winds

We have calculated a basic grid of frequency-dependent dynamical models (Höfner et al. 2002b) to demonstrate the dependence of their properties on stellar parameters and pulsation, and to compare this new generation of atmospheres to existing grey models based on Planck mean gas opacities (Höfner et al. 1998).

Table 1. Model parameters ($L_\star$, $T_\star$, C/O, P, Δu_p; $M_\star = 1\,M_\odot$ for all models) and results (mass loss rate $\dot{M}$, mean velocity at the outer boundary $\langle u \rangle$). See text for explanation of symbols.

Model	$L_\star$ [$L_\odot$]	$T_\star$ [K]	C/O	P [d]	Δu_p [km/s]	$\dot{M}$ [$M_\odot$/yr]	$\langle u \rangle$ [km/s]
l70t28c14u2	7000	2800	1.40	390	2.0	–	–
l70t28c14u4	7000	2800	1.40	390	4.0	$2.4 \cdot 10^{-6}$	11
l10t28c14u4	10000	2800	1.40	525	4.0	$2.5 \cdot 10^{-6}$	14
l10t28osu2	10000	2800	0.48	525	2.0	–	–

Regarding their dynamical behaviour, the C-rich models form two groups: If the effective temperature of the star is too high, the C/O ratio is too low, or if the levitation (dynamic enhancement of the density in the outer layers) due to pulsation is not sufficient, no dust will form. After a transient phase of adjusting from the initial hydrostatic structure the dust-free models settle into a periodic dynamical behaviour. During each pulsation period a strong radiating shock wave forms and propagates outwards through the atmosphere. After a layer is hit by a shock wave it follows a roughly ballistic trajectory and returns to its initial position before being hit by the next shock wave. On the other hand, if the densities of condensible material in the cool outer layers are high enough to allow for grain formation, an outflow driven by radiation pressure on dust evolves. The dust formation process – which proceeds far from equilibrium – has its own time scales which do not necessarily agree with the pulsation period or the acceleration time scale of the wind. Therefore, complex multi- or non-periodic patterns may occur in the spatial structures, depending on the stellar parameters.

The O-rich models show a similar division concerning their dynamical properties, depending on whether a sufficiently high parameterized dust opacity is included or not. However, in this case the dust opacity is just a simple function of the temperature (see Sect. 2.1.), and therefore it adjusts instantaneously to the conditions in the atmosphere which leads to a much simpler temporal behaviour of the wind models.

2.3. Effects of frequency-dependent radiative transfer

Comparing the hydrostatic limit case of our models to atmospheres calculated with the MARCS code (Gustafsson et al. 1975, version of Jørgensen et al. 1992 with spherical radiative transfer routines from Nordlund 1984) which are based on the same molecular opacities, we find that our models resemble the temperature-pressure structure of the MARCS models quite closely, in spite of the small number of frequency points used in the radiative transfer. In contrast,

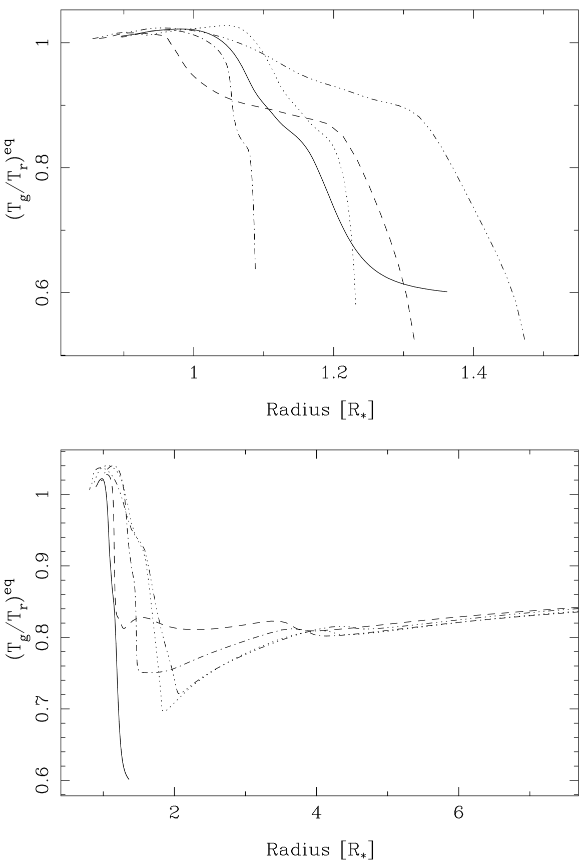

Figure 1. Ratio of the radiative equilibrium gas temperature to the radiation temperature as a function of the radius coordinate (in units of the stellar radius of the hydrostatic initial model $R_\star$) for different phases of dynamical models and for the corresponding hydrostatic initial model (full line); upper panel: model l70t28c14u2, lower panel: model l70t28c14u4; see Tab. 1 for the stellar parameters of the models.

grey models using, e.g., Planck means of the same opacity data tend to severely underestimate the density at a given temperature in the outer layers of the atmosphere, due to frequency-dependent effects like line blanketing by molecules which cannot be simulated with mean opacities (cf. Höfner et al. 1998, Höfner 1999).

To demonstrate the non-grey effects in dynamical models we have plotted the ratio of the radiative equilibrium gas temperature (which differs from the actual gas temperature in shock waves) to the radiation temperature (which corresponds to the energy density of the radiative field) as a function of the radius in Fig. 1. For a grey model, by definition, this ratio would be unity everywhere. The non-grey models, however, show strong deviations from this value in the outer atmospheric layers due to the influence of molecular opacities. The complex molecules forming in the cooler layers above the photosphere absorb mostly in the near- and mid-infrared, i.e. at wavelengths larger than the flux maximum, leading to a significant cooling of these layers below the radiation temperature (up to several hundred Kelvin). The upper panel shows model l70t28c14u2 (see Tab. 1) which does not form dust and has no stellar wind. The lower panel shows model l70t28c14u4 which differs from the upper one by a higher pulsation amplitude (Δu_{p}; cf. Tab. 1) and has a well-developed dust-driven wind (see Höfner et al. 2002b for details). The overall non-grey effects are somewhat smaller for the model shown in the lower panel but the maximum deviation in the wind model occurs around two stellar radii, in the zone where dust formation starts and a significant part of the infrared molecular features are formed. Therefore the frequency-dependent treatment of radiative transfer has a considerable influence both on the resulting spectra and the stellar wind.

The non-grey effect on the temperature of the amorphous carbon grains is somewhat smaller (typically 200 K) but goes into the opposite direction. Since the extinction coefficient of the grains is inversely proportional to the wavelength (cf. Fig. 2 in Andersen et al., this conference) the grains are hotter than the radiation field, and significantly hotter than the surrounding gas. In addition to its effects on the temperatures of gas and dust grains the frequency-dependent description of radiative transfer also influences the momentum balance of the atmosphere and wind, mainly through the radiative pressure on the dust grains. The radiative pressure is accelerating the outflow more efficiently in the new frequency-dependent C–star models in comparison with the grey wind models presented by Höfner et al. (1998).

2.4. Influence of dust grain properties

It is considered as relatively certain that a major part of the dust in C-rich AGB stars consists of amorphous carbon (as opposed to graphite which has spectral features that are absent in AGB stars). The term amorphous carbon however is problematic, since it summarizes a whole range of materials with different ratios of chemical bonds. These different types of amorphous carbon may have quite different optical properties as demonstrated by laboratory studies (cf. Andersen et al. 1999 for an overview). As discussed above, the carbon grains have a strong influence on the structure and wind properties of dynamical models due to their high opacity compared to the gas. It is therefore important to use the right material properties, or at least to select consistent values for the different quantities which describe the grain material in the models.

The wavelength dependence of the grain extinction efficiency determines both, the radiative equilibrium grain temperature and the radiation pressure on dust which is the main source of momentum for the stellar wind. Materials classified as amorphous carbon have an extinction efficiency which is inversely proportional to the wavelength with exponents of about -1 to -2 in the relevant spectral region around the flux maximum. The steeper the dependence on wavelength, the larger the difference between the equilibrium grain temperature and the radiation temperature. The radiative pressure on the other hand is proportional to the flux mean opacity which both depends on the slope of the extinction efficiency as a function of wavelength and on its absolute value. The latter may differ by almost an order of magnitude for different types of amorphous carbon in the critical region around 1 μm.

The optical properties of the grain material are only the most obvious microphysical quantities which enter the models. As we have mentioned above, dust formation usually proceeds far from equilibrium. Therefore we have to calculate the rates at which grains are formed out of the gas (nucleation) and at which new material is added to existing grains (grain growth). This requires material-dependent input data in the form of the density of the grain material (which is also relevant for calculating the opacity and has to be chosen consistently with the grain extinction efficiency), the surface tension of the grain material, and the so-called sticking coefficients, i.e. the probabilities that atoms and molecules which hit a grain will stick to the surface.

Andersen et al. (2002 and this conference) have investigated the influence of these quantities on the dynamical models described here and found that even a moderate variation of the values within the range expected for possible materials has noticeable consequences for the properties of the dust–driven stellar winds, including the resulting near-IR colors. In some cases, the choice of the type of amorphous carbon actually makes the difference if a wind will develop at all, or not, for given stellar parameters.

2.5. Drift between gas and dust

In the models which we have discussed so far, we have tacitly assumed that gas and dust move with the same speed. This, however, is not necessarily the case in a dust-driven stellar wind. Dust grains – in particular those consisting of amorphous carbon – absorb radiation more efficiently than the gas and rapidly gain momentum due to their small total mass. This outwards-directed momentum is transferred to the gas through gas–grain collisions. The efficiency of the momentum transfer depends on the frequency of the collisions, and thus on the number densities of the gas and dust particles, and their relative velocities. This means that gas and dust may move with different velocities, i.e. drift relative to each other while moving away from the star. Furthermore, possibly only a part of the momentum gained by the grains through radiative acceleration is transfered to the gas, not all of it, as often assumed in wind models.

The phenomenon of drift as such has been discussed in the context of dust-driven stellar winds for decades but it has only been included in time-dependent dynamical models rather recently (cf. Simis et al. 2001 and references therein). Nevertheless, it seems important to study the dust-gas coupling in detail since it is crucial for the formation of dust-driven winds.

Sandin & Höfner (2002 and this conference) have included a separate equation of motion for the dust phase into an earlier grey version of the models discussed in this contribution, allowing for drift between gas and dust, and treating momentum transfer between dust and gas explicitly by drag force terms in the two equations of motion. These preliminary models are calculated without a variable inner boundary simulating stellar pulsation and permit to study the effects of drift in purely dust-driven winds without the influence of atmospheric levitation by pulsation. The main results of this study are that the extra degree of freedom provided by drift tends to increase dust-induced instabilities in the stellar winds and shifts the threshold of stellar parameters at which purely dust-driven outflows can form. Dust has the tendency to move from zones with low gas density to high gas density regions behind shock waves where the coupling

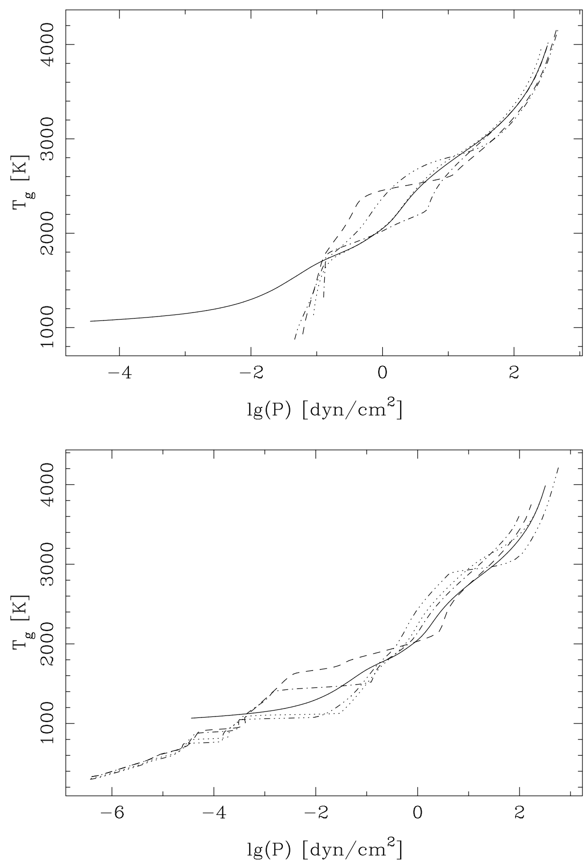

Figure 2. Pressure–temperature structures for different phases of dynamical models and for the corresponding hydrostatic initial model (full line); upper panel: model l70t28c14u2, lower panel: model l70t28c14u4; see Tab. 1 for the stellar parameters of the models.

between gas and dust is strong, enhancing the shell-like structure of the circumstellar envelopes. Currently, more realistic models which include both drift and stellar pulsation are under construction.

3. Comparison with observations

Like classical hydrostatic model atmospheres, dynamical models can be used to calculate various observable properties. At selected phases snapshots of the spatial structure are stored and they can be used later as input for more detailed radiative transfer calculations. The densities, temperatures, velocities, etc., resulting from the radiation–hydrodynamical simulation are the basis for computing opacities and solving the radiative transfer equation at the desired spectral resolution. Below, we give an overview of synthetic observable properties of our models, from IR colors to high-resolution spectra which allow to study line profile variations due to the velocity fields in the atmospheres.

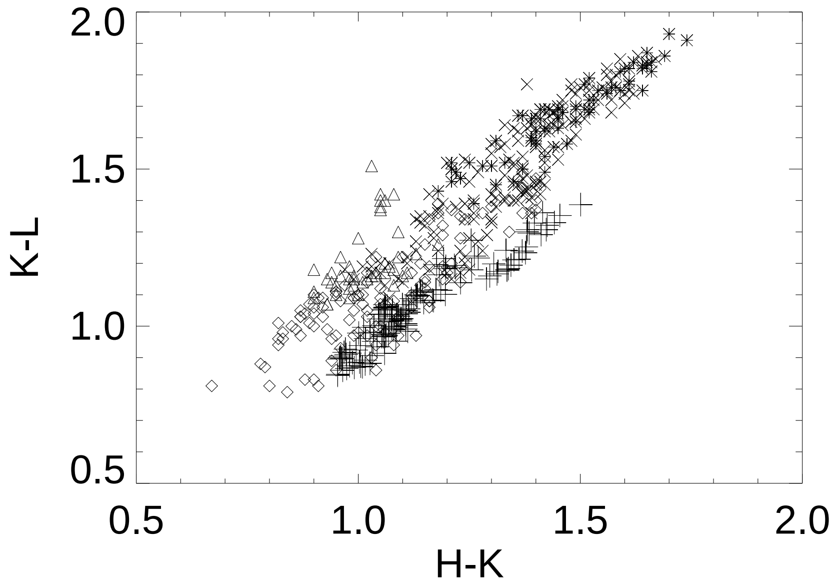

Figure 3. Infrared colors of dynamical models (+) and of C-rich Miras with comparable mass loss rates; V Hya (triangles), R Vol (stars), R For (crosses) and R Lep (diamonds). From Andersen et al. (this conference).

3.1. Low-resolution spectra and IR colors

The propagating shock waves resulting from stellar pulsation cause step-like features in the atmospheric pressure–temperature structures (see Fig. 2). These variations can not be described in a consistent way by series of hydrostatic models with different stellar parameters. In particular, the need for dynamical model atmospheres has become apparent with the analysis of ISO-SWS spectra which show a combination of features originating in different layers, including both the photospheric region and the transition zone to the stellar wind.

The grey dynamical models based on Planck mean molecular opacities presented in Höfner et al. (1998) differ from frequency-dependent models by a systematically lower gas density at a given temperature in the inner parts of the atmospheres, caused by an over-estimation of the radiative pressure on the gas. Therefore, the overall spectral energy distributions of these grey models are unrealistic, with the maxima shifted to shorter wavelengths. Nevertheless the models could be used for preliminary studies of the qualitative variations of IR molecular features in ISO-SWS spectra (e.g. Hron et al. 1998).

Due to the improved pressure–temperature structure, the new frequency-dependent models show energy distributions and near-IR colors in good agreement with observations (see Fig. 3). The new models are able to reproduce the observed low-resolution spectra of C stars reasonably well between 0.5 and 5 μm and are similar to synthetic spectra calculated from MARCS models in the hydrostatic limit. At wavelengths longer than 5 μm, however, some of the dynamical models show emissions of certain molecular features which are not

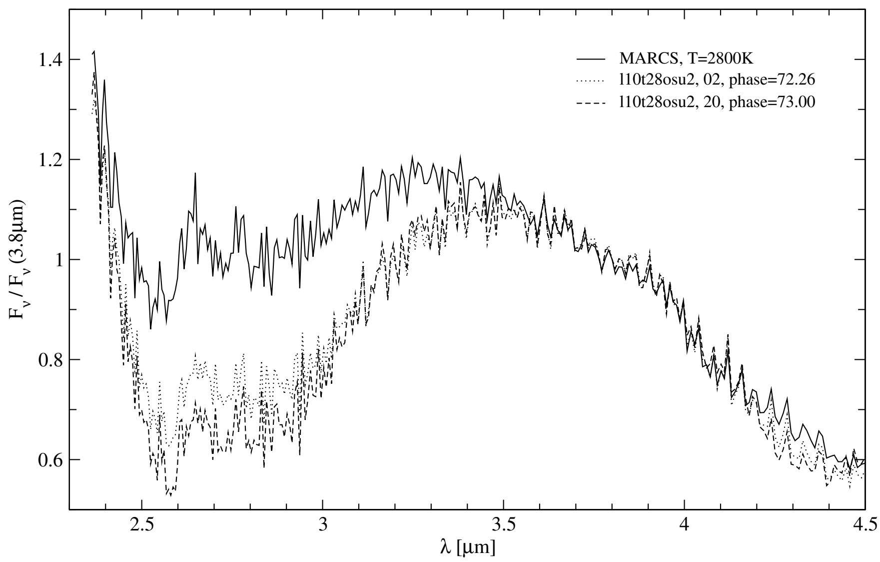

Figure 4. Spectra calculated from two phases of the non-grey atmosphere l10t28osu2 and from the corresponding MARCS model (same parameters as the initial model). All spectra are normalized to the flux at 3.8 μm where the molecular opacity has a minimum and the resolution is set to 450.

observed (this problem is still under investigation). Synthetic spectra of C-stars in the ISO-SWS range and comparisons to observations can be found, e.g., in Loidl et al. (2000), Höfner et al. (2000, 2002b) and in the contribution of Hron et al. (this conference).

Aringer et al. (2002 and this conference) have recently studied H_2O features in the 2.5 μm region and SiO bands at 4 μm using ISO-SWS data. Different groups of AGB stars can be fitted to a varying degree with MARCS models: The spectra of the investigated semiregular variables are reproduced by the models, with the exception of SiO first overtone bands around 4 μm in stars with an effective temperature below 3000 K. There is however a persistent problem to fit the deep water absorption of Miras, especially around minimum light, which has led Aringer et al. (2002) to claim that this situation can only be resolved with dynamical models.

Figure 4 shows spectra calculated from two phases of the non-grey atmosphere l10t28osu2 and from the corresponding MARCS model (same parameters as the initial model). For the dynamical model, the water features are more intense than for the hydrostatic MARCS model, in significantly better agreement with the observations. It should be noted that the used model still cannot reproduce the deep water depression observed by Aringer et al. (2002) or Matsuura et al. (2002) in Mira variables around minimum light. This, however, may be due to the parameters of the chosen model. Currently, we are performing a more detailed study of our O-rich models regarding the water features.

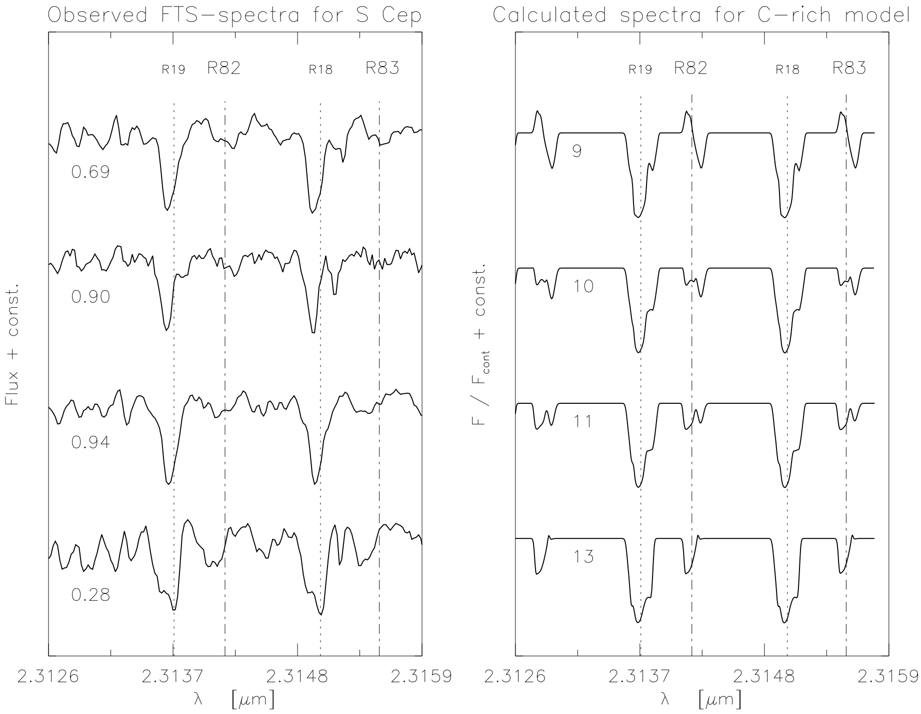

Figure 5. Time-dependent behaviour of CO first overtone lines. Observed spectra of S Cep (left) and synthetic lines resulting from the dynamical model l10t28c14u4 (right). See Nowotny et al. (this conference) for details.

3.2. Line profile variations

The complex velocity fields caused by shock waves and radiative acceleration lead to intricate variable profiles of molecular lines. One of the most well-known phenomena is the doubling of CO lines around the luminosity maximum (e.g. Hinkle et al. 1982) which is interpreted as a shock front crossing the line formation zone, splitting the line into two parts, one formed in front of the shock and one behind the shock. Among the many molecules which are present in atmospheres of AGB stars, CO plays a special role: it is abundant both in M and C stars and has many observable transitions which allow to probe different layers of the atmospheres and winds.

Given the complicate structure of the atmospheres, the most reliable way of interpreting observed time series of high-resolution spectra seems to be a comparison with synthetic line profiles resulting from self-consistent dynamical models. We have recently started to calculate profiles of CO lines based on our latest generation of dynamical models. First results are presented in the contributions of Nowotny et al. and Lebzelter et al. (this conference). Selected snapshots of the structure of model l10t28c14u4 (see Tab. 1) are used as input for a spherical radiative transfer code which takes the Doppler shifts caused by the velocity field into account. The resulting CO first overtone lines at 2.3 μm

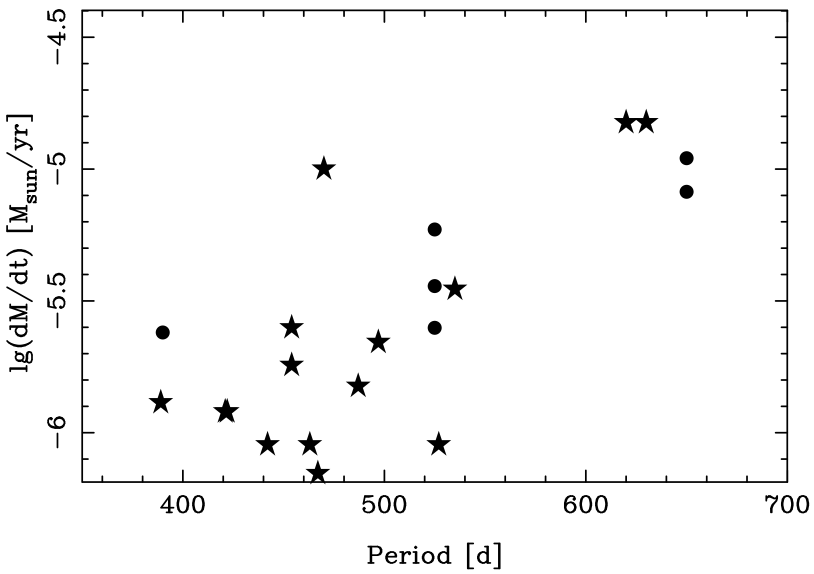

Figure 6. Mass loss rate vs. pulsation period: full circles correspond to the models presented by Höfner et al. (2002b), stars to values derived by Schöier & Olofsson (2001) from observations of C-rich Miras.

(see Fig. 5) show a qualitative agreement with observations of the C-rich Mira S Cep which has comparable stellar parameters (no detailed fit was attempted). This preliminary result makes us confident about the diagnostic power of this method to study the kinematics of Mira atmospheres and winds. Further studies are currently performed.

4. Conclusions

To understand atmospheres of pulsating AGB stars, it is essential to include time-dependent dynamics in the models. Dynamical processes influence the atmospheric structures both on local and global scales through propagating shock waves and stellar winds. Sequences of hydrostatic models with different stellar parameters cannot reproduce these effects. Only dynamical models permit to study temporal variations of observable properties like colors or line profiles, and mass loss by stellar winds in a consistent way.

A frequency-dependent treatment of radiative transfer in such dynamical models is crucial for obtaining realistic structures and synthetic spectra, as well as reliable mass loss rates. The use of grey opacities leads to systematically wrong global pressure–temperature structures which affects the resulting spectra and consequently the interpretation of observed data. The new generation of dynamical models discussed in this contribution represents an important step in a transition from qualitative to quantitative modelling, as demonstrated by comparisons with MARCS models and observations.

Current and future projects include studies of the influence of microphysical input data, in particular for dust, and of the effects of drift between gas and dust. We are in the process of exploring the variability of observable properties and their dependence on stellar parameters to obtain a detailed interpretation of observations for individual AGB stars (IR-spectra, line profiles, colors, etc.).

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