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Dynamical models of LPV atmospheres: a comparative study

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Abstract. Numerical models for atmospheres of carbon–rich long-period variables (LPVs) obtained by two different codes are compared with regard to the radial structure of the circumstellar shell, its dynamics and the propagation of shock waves, the dust formation and its effects on the dynamics and thermodynamics of the atmosphere as well as the mass loss rates and the outflow velocities. The general features of the models such as the formation of discrete dust layers, the occurrence of multiperiodicity or the dust-induced κ-mechanism in purely dust-driven winds are the same in both cases while a detailed quantitative comparison of special model calculations demonstrates certain effects caused by the different numerical schemes. Nevertheless we find that the two modelling methods give remarkably similar results with respect to the complex physical system under consideration.

Key words: hydrodynamics – shock waves – methods: numerical – stars: circumstellar matter – stars: AGB and post–AGB

1. Introduction

Numerical investigations of astrophysical problems often suffer from the fact that the internal computational errors cannot be estimated. Usually, extensive numerical codes are compared to analytical solutions of physically rather simple problems although the relevant astrophysical results are then calculated with a completely different physical input, initial and boundary conditions. If such computations lead to direct observational predictions it is essential to disentangle the uncertainties of the input physics from numerical insufficiencies.

A possible solution of this problem is to compare the results of two numerically entirely different codes for the same astrophysical situation, i.e. in our case for the dynamics of an extended atmosphere around a long-period variable (LPV). In these objects the levitation of the atmosphere by the dissipation of running shock waves together with radiation pressure on newly formed dust grains provide an effective mechanism for the generation of outflows with low terminal velocities but high mass loss rates. To achieve a comprehensive understanding of the physical processes in these circumstellar shells, hydrodynamics, radiative transfer, chemistry as well as dust formation, growth, and evaporation have to be taken into account simultaneously.

During the last few years two groups in Berlin and Vienna have developed extensive codes based on completely different numerical schemes to calculate dynamical models of LPV atmospheres which include a time-dependent description of the dust component. The modelling results presented in various publications demonstrate that the general features of the models are quite similar. However, we are now interested in a more detailed comparison of model calculations which may show the effects of the different numerical schemes and, consequently, help to test the reliability of the results.

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2. Modelling methods

Since both modelling methods have been presented in detail in earlier publications (Berlin: Fleischer 1994, Fleischer et al. 1991, 1992, 1995; Vienna: Dorfi & Höfner 1991, Höfner & Dorfi 1992, Feuchtinger et al. 1993; Höfner 1994, Höfner et al. 1995), we only give a brief summary here concentrating on the differences concerning the input physics and numerics and refer the reader to the papers mentioned above for general information. To allow a simple distinction we call these methods either the *Berlin* or the *Vienna* approach.

2.1. Input physics

Both codes solve the coupled system consisting of the equations of hydrodynamics, the equations of dust formation and growth and grey radiative transfer. Apart from the formulation of the equations (differential vs. conservation form) hydrodynamics is treated identically in both codes and also the description of dust formation and growth according to the moment method developed by Gail & Sedlmayr (1988) and Gauger et al. (1990) is equal. We consider the formation and growth of amorphous carbon grains using an equilibrium chemistry to determine the number densities of the relevant chemical species.

In contrast to the equations for the gas and dust, the treatment of radiative transfer differs in the two codes. The Berlin approach uses the semi-analytical method of Lucy (1971, 1976) which yields a prescription for the radiative equilibrium temperature. To describe the energy exchange between the gas and the radiation field one can optionally make use of different cooling functions in the gas energy equation. The Vienna approach solves the time–dependent moment equations of the grey radiative transfer equation (which describe the energy and momentum balance of the radiation field) closing the system with a variable Eddington factor.

2.2. Numerical techniques

The *Berlin approach* is based essentially on the modelling method developed by Bowen (1988), which is well suited for the consistent incorporation of the dust equations, and which quickly allows modifications of the input physics. Adopting Lagrangian coordinates the basic equations are written in standard finite difference form and solved by explicit integration according to the scheme of Richtmyer and Morton (1967). Therefore the time steps are restricted by the Courant–Friedrichs–Levy (CFL) stability condition. Due to the Lagrangian description of the flow the radial grid might become too sparse, especially in the regions of acceleration by radiation pressure on dust. To keep the spatial resolution sufficiently fine a rezoning scheme of the radial grid is performed after constant time intervals, which in principle ensures conservation of physical quantities.

The *Vienna approach* (e.g. Dorfi & Feuchtinger 1995) is based on an implicit solution of the discretized equations, i.e. the system of nonlinear algebraic equations is iterated by a multidimensional Newton-Raphson procedure. In this case the time step is not restricted by the CFL-condition but given by accuracy demands and the convergence radius of the iteration. Furthermore, an additional so-called grid equation (Dorfi & Drury 1987) which determines the actual location of the grid points in order to achieve an optimal resolution for relevant physical quantities is solved simultaneously with the physical equations. Hence, this method uses neither an Eulerian nor a Lagrangian representation of the physical equations but requires a formulation appropriate for an adaptive grid. To ensure an overall conservation of global quantities (mass, momentum, energy) a so-called conservative discretization is employed and the advection across cell boundaries is done by a monotonic 2$^{\rm nd}$-order scheme according to van Leer (1977). Both methods use a tensor viscosity (Tscharnuter & Winkler 1979) to broaden shock fronts over a finite number of grid points.

3. General model characteristics

Probably the most important feature of models including a self-consistent time-dependent treatment of dust formation and growth – in contrast to the pioneering model calculations by Wood (1979) and Bowen (1988) which consider the influence of dust in the form of an additional parameterized opacity only – is the formation of discrete dust layers associated with strong shocks. This phenomenon is due to the complex interactions of dust formation and growth, hydrodynamics and thermodynamics as described in detail by Fleischer et al. (1991, 1992).

A similar mechanism is responsible for an instability occuring in certain models of stellar winds driven by radiation pressure on dust alone, i.e. models without a piston simulating the stellar pulsation. This dust-induced κ-mechanism leads to a (more or less) periodic formation of dust and creation of shock waves instead of a stationary outflow and has been investigated by Fleischer et al. (1995) and Höfner et al. (1995).

Due to the fact, that both modelling methods include a time-dependent description of the dust component a periodic inner boundary condition (piston) does not guarantee a periodical behaviour of the circumstellar envelope on the time scale of the piston. In fact such a behaviour (in the following referred to as single-periodic) is obtained only for very special combinations of the parameter values. So–called *multiperiodic* models have been presented e.g. in Winters et al. (1994). In these models the dynamics and dust formation in the circumstellar shell repeats on a time-scale that is an integer multiple of the piston period. However, even this more generally defined periodicity is only found for certain combinations of physical parameters. In general, models including a time-dependent description of dust formation will not show a periodical behaviour of the circumstellar shell at all (e.g. Winters et al. 1995).

4. Detailed comparison of model calculations

In the following we present a quantitative comparison of Berlin and Vienna models especially calculated for this purpose by adjusting physical and numerical parameters.

4.1. Model parameters

As a starting point for our investigations we use Model E (in the following referred to as E92) of Fleischer et al. (1992) – a single-periodic model which has been discussed and plotted in detail and also has been used for radiative transfer calculations by Winters et al. (1994, 1995; IR light curves and brightness profiles). The corresponding parameters of the hydrostatic initial model are $M_\star = 1 M_\odot$, $L_\star = 10^4 L_\odot$, $T_\star = 2600$ K and $\varepsilon_{\rm C}/\varepsilon_{\rm O} = 1.8$ together with the following piston parameters: period $P = 650$ d, velocity amplitude $\Delta u_{\rm p} = 2.0$ km/s and initial position of the inner boundary $R_{\rm in}(t=0) = 0.91 R_\star$ (≈ 2 pressure scale heights below the photosphere).

To ensure a better comparability with the Vienna models the Berlin calculations presented here have been performed with LTE cooling (instead of isothermal shocks), the radiative flux at the moving inner boundary was kept constant (instead of $T_{\rm eff}$ = const) – leading to a variation of the luminosity at the inner boundary $L_{\rm in}(t) \propto R_{\rm in}(t)^2$ – and the models include self-gravity.

Table 1. Comparison of results (B: Berlin, V: Vienna models): mass loss rate $\dot{M}$, velocity at the outer boundary u_∞ and dust-to-gas mass ratio ρ_d/ρ_g. $P_{\rm dyn}$ and $P_{\rm dust}$ are periods (in units of the piston period P) characterizing the dynamics of the circumstellar envelope and the formation of new dust shells, respectively. Parameters: $M_\star = 1 M_\odot$, $L_\star = 10^4 L_\odot$; piston period P = 650 d (except models BS and VS); effective temperature $T_{\rm eff}$, carbon abundance $\varepsilon_{\rm C}/\varepsilon_{\rm O}$, piston velocity amplitude $\Delta u_{\rm p}$, characteristic length scale of the artificial viscosity $\ell_{\rm AV}$.

model	$T_{\rm eff}$ [K]	$\varepsilon_{\rm C}/\varepsilon_{\rm O}$	$\Delta u_{\rm p}$ [km s^{-1}]	$\ell_{\rm AV}$	$\dot{M}$ [$M_\odot$ yr^{-1}]	u_∞ [km s^{-1}]	ρ_d/ρ_g [10^{-3}]	$P_{\rm dyn}$ [P]	$P_{\rm dust}$ [P]
BS	2600	2.3	0.0	2.5 Δr	1.8 10^{-7}	11	1.5	–	–
B1	2600	1.8	2.0	2.5 Δr	0.8 10^{-5}	25	4.3	1	1
B2	2600	1.8	2.0	7.5 $10^{-3} R_\star$	1.4 10^{-5}	24	3.9	2	1
VS	2600	2.3	0.0	3.5 $10^{-3} r$	2.9 10^{-7}	12	1.5	–	–
V1	2600	1.7	2.0	3.5 $10^{-3} r$	2.6 10^{-5}	22	3.1	2	1
V2	2745	1.8	2.0	3.5 $10^{-3} r$	1.0 10^{-5}	25	3.6	1	1
V3	2600	1.8	2.0	7.5 $10^{-3} R_\star$	2.2 10^{-5}	24	3.5	2	1

4.2. Purely dust-driven winds

First, to avoid the complications associated with the treatment of strong shock waves (cf. Sect. 4.3), we want to compare models of stellar winds which are calculated without a variable inner boundary simulating the stellar pulsation. Adopting the stellar parameters of Model E92, but without a piston that enhances the gas density ($\Delta u_{\rm p}$ = 0.0), a relatively high carbon/oxygen abundance ratio of $\varepsilon_{\rm C}/\varepsilon_{\rm O}$ = 2.3 is necessary to drive an outflow at a reasonable speed.

After a short transition phase from the dust-free (but supersaturated) hydrostatic initial model to a dust-driven outflow the Vienna model reaches a stationary state. In contrast to that the Berlin model shows slight temporal variations, i.e. small waves associated with changes in the degree of condensation. The variability is caused by the dust-induced κ-mechanism (cf. Fleischer et al. 1995, Höfner et al. 1995) which is relatively weak in this model but nevertheless present for the parameters chosen.

This difference between the models is a direct result of the numerical methods. In the explicit Berlin approach the time step is limited by the CFL condition and therefore remains small throughout the calculation. In the implicit Vienna code it is chosen according to the temporal variations of the variables and is in general much larger. Thus in the Berlin model the κ-mechanism is activated by small amplitude perturbations while in the Vienna model the effects of the transition phase have been damped out due to the much larger time steps. A second reason for the perturbations occurring in the Berlin model is the necessity of using a rezoning scheme in the Lagrangian description to redistribute the grid points (cf. Sect. 2.2). Although carefully done, this scheme introduces additional perturbations, which can be avoided *without* rezoning at the price of a too sparse grid.

The mass loss rate $\dot{M}$, outflow velocity u_∞ and dust-to-gas mass ratio ρ_d/ρ_g of the two models (VS, BS) are given in Tab. 1. We see that the fraction of material condensed into grains is the same in both cases and the outflow velocity differs only sightly. The values of the mass loss rates probably reflect the differences in the radiative transfer and its consequences for the temperature and density structure of the models.

4.3. Piston models

Choosing the parameters of model E92 (cf. Sect. 4.1) we have performed a new calculation with the Berlin code – model B1 – to demonstrate the effects of the modified input physics employed here. The mass loss rate, outflow velocity and dust-to-gas mass ratio do not change significantly compared to model E92 and we still get a single-periodic solution. However, every attempt to obtain a single-periodic Vienna model with the same physical parameters failed. First, interpreting this as a consequence of the physical differences in the modelling methods, we have tried to construct a periodic Vienna model by varying the physical parameters of the initial model, one at a time.

Calculating a series of Vienna models with different values of $\varepsilon_{\rm C}/\varepsilon_{\rm O}$ we obtain a multiperiodic model (V1) with $\varepsilon_{\rm C}/\varepsilon_{\rm O}$ = 1.7 but no single-periodic model. In this model the dynamics of the circumstellar envelope repeats on a time-scale of two piston periods ($P_{\rm dyn}$ = 2 P) while a new dust shell is formed once each piston period ($P_{\rm dust}$ = 1 P). Alternately, the formation of a new dust layer is triggered by a shock wave (as in the single-periodic model B1) and spontaneous (in the wake of the preceeding dust layer, above the dust-free shock wave created by the pulsation). Apart from this multiperiodic behaviour it is interesting to notice that the mass loss rate of model V1 is significantly higher than in model B1. This fact in combination with the spontaneous formation of dust shells (i.e. without the presence of a density-enhancing shock wave) every second piston period leads to the conclusion that the mean density in the dust formation region – which is also the acceleration zone of the stellar wind – must be higher than in model B1.

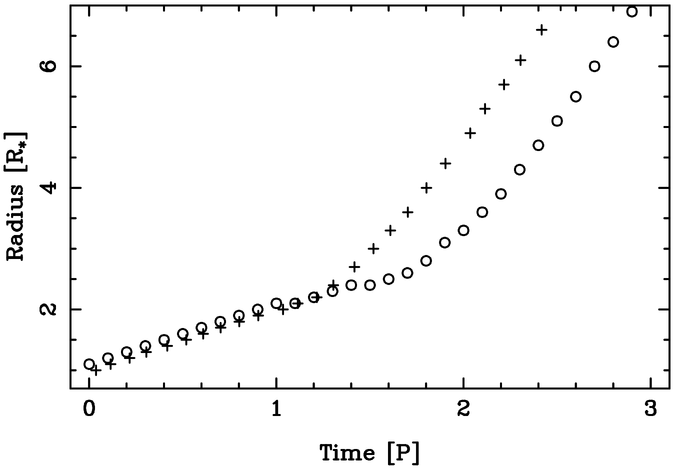

Fig. 1. Propagation of shock waves for model B1 (circles) and V2 (crosses): time in piston periods P, radius in units of the stellar radius $R_\star$ of the hydrostatic initial model with $T_{\rm eff}$ = 2600 K (i.e. 493 $R_\odot$).

The next attempt is to obtain a single-periodic Vienna model by adjusting the effective temperature of the initial model which strongly affects the density structure of the atmosphere and thus may help to compensate the differences compared to model B1. Calculating a series of models with different effective temperatures we actually find a single-periodic model (V2) with $T_{\rm eff}$ = 2745 K. Though both models V2 and B1 are single-periodic and their mass loss rates and outflow velocities are comparable (Tab. 1) there is one striking difference: although the shocks are created at the same phase of the piston cycle, the time interval, that passes before the dust formation is triggered by a particular shock wave, is considerably longer in model B1. Thus relative to the piston period the dust cycle in model B1 is phase-shifted by about 0.5 P compared to model V2. Since observable properties like near-IR light curves are strongly influenced by the dust formation (e.g. Winters et al. 1994) we have to investigate this effect and its possible causes.

In Fig. 1 we have plotted the position of a single shock wave as a function of time for each of the two models into one diagram. The propagation of the two shocks is almost identical until the dust formation begins in model V2. Then the shock wave in model V2 (crosses) is enhanced and accelerated by radiation pressure on the dust and overtakes the shock of model B2 (circles). Approximately half a piston cycle later dust formation takes place in model B2 leading to an acceleration of the shock wave and afterwards both shocks run almost parallel again reaching the same radial positions with a phase difference of about half a piston period.

Both, this phase shift and the mass loss rate, seem to indicate that the mean density in model B1 is lower than in model V2 though the opposite is true for the corresponding initial models. Since the density in the dust formation zone is mainly controlled by the shock waves we have to discuss the numerical treatment of the shocks and the dissipational effects inherent to the numerical schemes. Two closely related problems in this context are the spatial resolution provided by the numerical schemes and the artificial viscosity.

Finite difference methods use an artificial viscosity (cf. Sect. 2.2) to spread shock fronts over several cells of the numerical grid. On the one hand the characteristic length scale $\ell_{\rm AV}$ of this artificial viscosity must be smaller than the physical length scales involved (e.g. the pressure scale heights) but on the other hand the resolution provided by the numerical grid is more or less limited. The Berlin code with its Lagrangian grid does not resolve the shock front and the radiative cooling zone very accurately while the adaptive grid of the Vienna code reaches high point concentrations in these regions (Note, however, that the advection across the cell boundaries of the adaptive grid has to be handled carefully and that certain minor advection problems arise in the outer parts of the models).

Model B1 has been calculated with $\ell_{\rm AV}$ proportional to the local grid spacing Δr as all other Berlin models described in earlier papers. This prescription of $\ell_{\rm AV}$ is dangerous: the value of the artificial viscosity is determined by the actual local grid spacing and changes instantaneously in the rezoning process.

In contrast, the Vienna code works the other way round: the grid spacing is controlled by a given viscosity via the velocity profile of shocks. The Vienna models V1 and V2 presented above have been calculated with $\ell_{\rm AV}$ being proportional to the local radius, i.e. the artificial viscosity increasing outwards (to avoid problems with too high grid point concentrations when a shock wave propagates across the outer boundary) but *not* depending on the grid spacing.

The lag of the dust condensation in model B1 which causes the phase shift relative to model V2 probably is due to the prescription of $\ell_{\rm AV}$ employed in the Berlin model. In the wake of the innermost dust layer the Lagrangian grid becomes sparse due to the radiative acceleration of the material and the fast outflow. Thus $\ell_{\rm AV}$ is increased, the next shock wave – running into a zone of higher artificial viscosity – is relatively weak and ineffective in compressing the gas and at first no dust formation takes place. Later, during the rezoning (which is performed every 0.5 P) the introduction of new grid points into the dust formation zone possibly triggers the onset of dust formation by locally reducing Δr and, consequently, $\ell_{\rm AV}$ thus leading to a steepening of shocks in this region.

To test this hypothesis we have performed a number of calculations with both codes using several fixed values of $\ell_{\rm AV}$ (independent of the local grid spacing Δr or the radius r) and the physical parameters of model E92. Though again we have not been able to obtain a single-periodic Vienna model with the same physical parameters as the E92/B1 model a multiperiodic model (V3) has been found during these tests. Model V3 is qualitatively quite similar to model V1 both concerning the dynamics of the circumstellar envelope and the mass loss rate.

On the other hand the new prescription of $\ell_{\rm AV}$ leads to considerable changes in the Berlin model (B2) compared to model B1. The mass loss rate increases significantly. The shock fronts are steeper and the temperature peaks are more pronounced. The formation of dust layers is alternately triggered by a shock and spontaneous as in the models V1/V3 and no lag of the onset of dust formation is discovered as in model B1. Note, however, that the mass loss rate (which is interpreted as an indicator of the mean density in the wind formation region) is still lower than in the comparable model V3.

This may be due to the different spatial resolution of the two schemes. While the prescribed value of $\ell_{\rm AV}$ in the new Berlin model B2 is equal to the value used in model V3 and does not depend on the grid spacing, the spatial resolution of the Berlin model itself has become worse regarding the steeper shock fronts and more narrow radiative cooling zones. Then, if the actual numerical dissipation of the Berlin code is controlled by the spatial resolution of the shocks rather than by the specified length scale of the artificial viscosity it would be larger than in the Vienna code. This might also explain the fact that for Berlin models with a spatially fixed $\ell_{\rm AV}$ the results depend only slightly on the actual value chosen and show no definite trends.

An alternative explanation is that we now are confronted with differences arising from the input physics. Note in this context, that the ratio of the mass loss rates of the models V3 and B2 is approximately the same as for the purely dust driven winds VS and BS (cf. Sect. 4.2 and Tab. 1).

5. Conclusions

The purpose of this paper is a comparison of two modelling methods used by the Berlin group and the Vienna group to describe the dynamical atmospheres of LPVs. The two numerical techniques are completely different but the input physics of the models is quite similar except for the treatment of radiative transfer. The calculations discussed in this paper help to estimate the reliability of our results.

A qualitative comparison of the models shows that the general features are the same in both types of models: the formation of discrete dust layers associated with strong shock waves, a complicated dynamical behaviour of the circumstellar shell on time-scales not necessarily associated with the piston applied at the inner boundary (e.g. multiperiodicity) or the instability of purely dust-driven winds due to a dust-induced κ-mechanism. A more detailed quantitative comparison demonstrates the effects of the different modelling methods.

First, in the case of an explicit scheme as employed in the Berlin code the time-step is limited severely by the CFL condition while in the implicit Vienna code it is controlled by the temporal variation of the physical quantities on the numerical grid and is in general much larger. This may lead to a situation where small-amplitude perturbations occurring on short time scales are ignored or damped by the Vienna code.

Secondly, the adaptive grid used in the Vienna code resolves certain features like steep shock fronts and narrow compressional heating and radiative cooling zones much better than the Lagrangian grid with periodical rezoning employed in the Berlin code. The rather limited spatial resolution of the Berlin method probably has a significant influence on the numerical dissipation of the scheme, especially in combination with the prescription of the characteristic length scale of the artificial viscosity employed in the original Berlin models which depends on the local grid spacing and has turned out to be problematic.

Using a spatially constant characteristic length scale of the artificial viscosity in both codes we have been able to obtain comparable piston models. This indicates that the numerical treatment of the shock waves plays a key role for the density in the dust formation region and, consequently, for the whole dynamics of the circumstellar envelope. The remaining quantitative differences may be due to other aspects of the numerical methods or to the input physics. By no means, however, one should overestimate these differences since the qualitative behaviour and the general features of the Berlin and Vienna models are remarkably similar with regard to the complexity of the physical system under investigation.

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