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Dynamical Modeling of Circumstellar Outflows

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Abstract. We review dynamical models of circumstellar dust shells around long-period variables which include time-dependent hydrodynamics and a detailed treatment of dust formation, growth and evaporation. Important effects caused by the complex interaction between the dynamics of the pulsating atmosphere and the dust complex which only can be revealed in the dynamical approach are summarized. Special emphasis is given to the treatment of the dust and gas opacity.

1. Introduction

In order to arrive at a realistic picture of an AGB outflow it has been shown that an appropriate model has to meet at least the following requirements (Fleischer et al. 1992; Höfner et al. 1996):

1. The hydrodynamical description has to be time–dependent, to describe the variations of the velocity field and the occurrence of shock waves caused by the pulsation of the central star.
2. Since the formation of dust is a crucial phenomenon in these objects, it is necessary to use a theory which describes the formation of solid particles depending on the physical conditions, and which does not prescribe essential quantities such as the site where the dust forms.
3. Furthermore, the chemistry of the gas phase has to be modeled in order to know at each instant of time and at each radial position how much condensible material is available.
4. Finally, it is mandatory to treat the radiative transfer problem in order to describe the influence of the radiation of the central object.

In contrast to the classical atmosphere problem, the presence of dust introduces a number of non-linear couplings and interactions which are of essential importance for the whole problem of an AGB outflow or, in general, for every outflow where phase transitions can take place. A reliable theoretical modeling on the one hand requires a *physical* description of the various ingredients, and on the other hand, at least equally important, it requires taking into account all interactions among the different physical components.

It is evident from the above list that the problem is non-linear and strongly coupled. If one considers for instance the coupling between hydrodynamics and

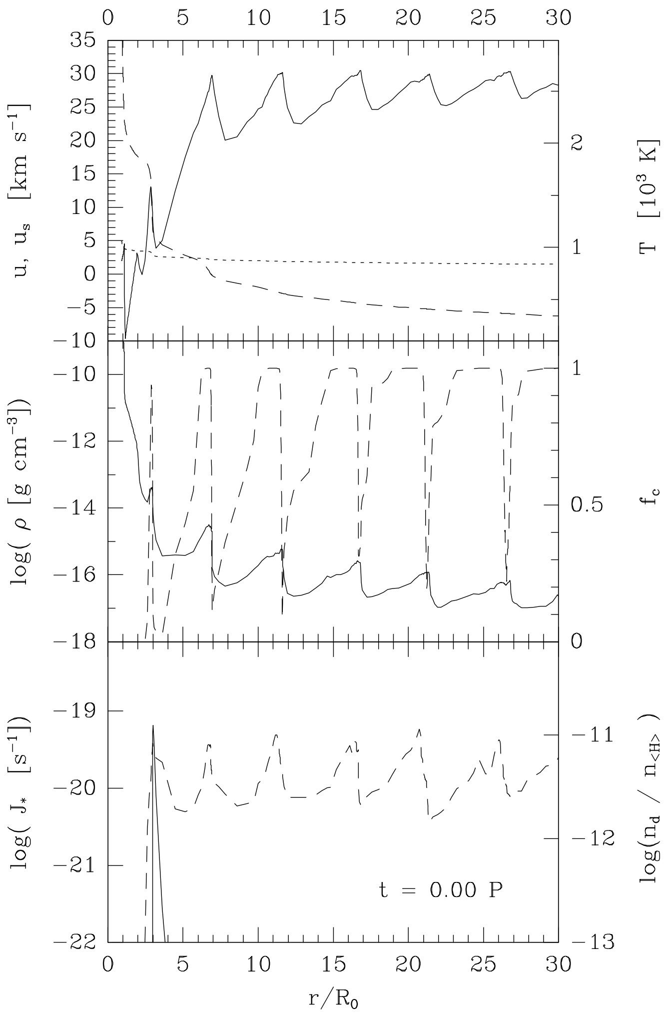

Figure 1. A typical radial structure of a dynamical model calculation

the dust complex: effective dust formation is possible only if the density is high enough; but at the same time, since radiation pressure on dust enters into the equation of motion, dust formation immediately influences the velocity structure, which in turn alters the density stratification.

The basic equations describing the dust forming circumstellar shell and the numerical methods applied for their solution are described in detail in Fleischer et al. (1992) and Fleischer (1994). These works deal exclusively with the case of carbon-rich circumstellar dust shells (CDS). First results concerning dynamical models of oxygen-rich CDS have been presented at this conference (Jeong et al., this volume). The pioneering works by e.g. Wood (1979) and Bowen (1988) give details about earlier research on this field.

For an introduction to the theory of dust formation we refer the reader to the series of papers by Gail and Sedlmayr. A good paper to start with is Gail & Sedlmayr (1986).

2. Phenomena revealed by the dynamical approach

The radial structure of a typical dynamical model is shown in Fig. 1. at the beginning of the pulsational period.

The parameters of this model are $L_\star = 1.0\ 10^4\ L_\odot$, $M_\star = 1.0\ M_\odot$, $T_\star = 2\,600\,K$, $\epsilon_C/\epsilon_O = 1.8$, P = 650 days, $\Delta u = 2$ km s^{-1}. In the following we refer to this set of parameters as our *standard* model.

It is evident from Fig. 1. that the dust is not distributed homogeneously across the shell but is concentrated in distinct layers such that the circumstellar dust shell exhibits an onion-like structure. Furthermore it can be seen that the dust quantities, e.g. the degree of condensation f_c (2^{nd} panel, dashed line), are intimately correlated with the hydrodynamical quantities, e.g. the velocity u (upper panel, solid line). This suggests that there is a common mechanism which produces this structure.

2.1. Re-amplification of the shock waves

A more detailed analysis shows that the shocks propagating through the atmosphere are not produced by the interior pulsation alone but are a product of the re-amplification of the pulsational shocks which is caused by the radiative acceleration α on dust grains in the discrete dust layers. The re-amplification is the result of a 2-step process: first, pulsational waves run into the region where initial dust nuclei are formed. They compress the material and initiate a phase of effective dust growth. Second, once a relevant amount of material has condensed into dust grains these grains become dynamically important. Radiation pressure on these newly formed grains amplifies the pulsational wave and dominant shock waves are formed which clearly can be seen in Fig. 1.

Since the radiative acceleration α exceeds unity close to the star, the material is accelerated to velocities above the escape velocity $v_{\rm esc}$ already at radii around $4\,R_*$ and a massive outflow is initiated. Details can be found in Fleischer et al. (1992).

2.2. Backwarming effect

Due to its opacity, the dust also leads to a pronounced heating of the material inside the dust layers (backwarming), as is evident from the steps present in the temperature stratification around $3\,R_\star$ and $6\,R_\star$ (upper panel, dashed line). The backwarming effect also introduces a new time scale into this dust-forming atmosphere (see Fleischer et al. 1995, Höfner et al. 1995, and Sect. 2.3). This can be inferred from the nucleation rate $J_\star$, the number of dust nuclei formed per second (lower panel, solid line). $J_\star$ has a sharp edge towards the star, caused be the high gas temperature, which prevents further nucleation. This high temperature is caused by the backwarming of the new dust layer which is also formed in this region. If this dust layer moves outwards the temperature behind the layer decreases and a new dust nucleation cycle may start.

2.3. Exterior κ-mechanism

Considering very luminous models of carbon-rich CDS a new nonlinear effect shows up which is caused by the dust opacity. Small amplitude waves are initiated in the innermost shell region by the backwarming. These waves provide the density enhancement necessary for a new dust formation and growth cycle. It can be shown that this mechanism already starts in an initially hydrostatic atmosphere and is self-maintaining in the dynamical model.

For these models, the CDS mimics a pulsating atmosphere, although this effect is solely caused by an instability due to the dust formation process.

Details about this phenomenon can be found in Fleischer et al. (1995).

2.4. Multiperiodicity

An important property of the model shown in the preceding section is that its radial structure repeats after *one* pulsational cycle.

For models calculated with the same parameter set as our standard model except with a reduced carbon overabundance, it turns out that the radial structure of the model repeats only after *two* pulsational cycles. Even tiny details of the radial structure, e.g. the multiple shocks present in the inner region below $4\,R_*$ in this model, are reproduced after this period of time. Around $2.5\,R_*$ at $t = 1.0\ P$ and $t = 3.0\ P$ in this model, a detailed analysis shows that the radiative acceleration α causes a pertubation in the velocity structure which later on turns into a dominant shock wave that sweeps up the preceding pulsational shock. Due to the reduced amount of condensable material it takes two pulsational cycles to form a new dust layer. The effect of *multiperiodicity* strongly depends on the ϵ_C/ϵ_O ratio. Lowering this number causes longer intervals between the formation of two dust layers; an increase causes the opposite effect. The time interval between the formation of two dust layers is of course not necessarily an integer multiple of the pulsation period, e.g. models with ϵ_C/ϵ_O values between 1.8 and 1.5 form a new dust layer on time scales larger than 1 and smaller than 2 pulsation periods. Depending on the remaining model parameters it is also possible that a dust layer forms on time scales of 3, 4, ... times the pulsation period, or even twice per pulsation cycle.

2.5. Deriving a mass loss formula

Based on a larger grid of dynamical models Arndt et al. (1997) were able to derive a fitting equation which relates a given set of the six model parameters to the resulting mass-loss rate. This formula reflects the strong dependence of the mass loss rate on the stellar mass and the stellar temperature.

Schröder et al. (1998) used this mass loss formula in stellar evolution calculations. They revealed an attractive mechanism which may lead to the formation of detached shells in the late stages of the AGB evolution. This finding was only possible by using a mass loss formula which is based on physical models in the relevant range of stellar parameters.

2.6. Infrared appearance of the dynamical models

The consistent treatment of the relevant physical processes also has profound influence on the IR-appearance of the models described above. We will not discuss here the occurring effects but refer the reader to the contribution of Winters et al. (1998, this volume) and e.g. to the recent paper of Winters et al. (1997).

3. Influence of the gas opacity

In the dynamical model calculations published so far, molecules have been treated only as a chemical pool for dust formation and growth. Radiation pressure on molecules has not yet been used as a supporting mechanism to drive the wind mostly because the investigations were aimed at dust-enshrouded objects. If dust is present it dominates the dynamics because the gas opacity, which is orders of magnitudes smaller, can be neglected. However, the question arises about the influence of radiation pressure on gas in less enshrouded objects and in the phase were the dust is initially forming. Höfner et al. (1998a, b) have pointed out that the gas opacity plays an important role in determining the near IR properties of these objects.

Very recently model calculations have been carried out by Helling (1998) in order to investigate the role of the gas opacity in more detail. From the opacity sampled line lists from the group of U. Jørgensen she computed mean opacities $\bar{\kappa}^{gas}$ for the two limiting cases of Planck and Rosseland opacities. These mean opacities were included into the hydro-code, replacing the previously used constant opacity.

Already in the initial hydrostatic model the influence of the gas opacity can be seen. The grey hydrostatic model atmospheres with $\kappa_H = \bar{\kappa}^{gas}_{Planck}$ are less dense than the hydrostatic models with $\kappa_H = \bar{\kappa}^{gas}_{Ross}$ which has profound consequences for the dynamical development of the model. Furthermore, models calculated with $\kappa_H = \bar{\kappa}^{gas}_{Planck}$ show a gas pressure inversion for certain combinations of stellar parameters which prevents effective dust formation in the corresponding dynamical model because the shocks caused by the interior pulsation cannot run into the region containing the dust nuclei but are damped already in the region of the pressure inversion. This effect does not occur in models with $\kappa_H = \bar{\kappa}^{gas}_{Ross}$.

For the parameters of the standard model which has been discussed in Fleischer et al. (1992) and in Sect. 2, the following quantities result for the two limiting cases:

Table 1. Resulting quantities of the evolved models for different mean gas opacities

	$<\dot{M}>$ $[M_\odot \mathrm{yr}^{-1}]$	$< v_\infty >$ $[\mathrm{kms}^{-1}]$	$\rho_\mathrm{d}/\rho_\mathrm{g}$
Planck mean	$1.5\,10^{-7}$	6.9	$4.8\,10^{-4}$
Rosseland mean	$4.3\,10^{-6}$	21.5	$2.4\,10^{-3}$

As a result of the pressure inversion in the "Planck models" the degree of condensation reaches only 15 % so that the mass loss rate and the final outflow velocity remain small. For the Rosseland mean the radial structure and the dynamics of the models are more or less similar to the ones described in Sect. 2.

To summarize, these calculations show that radiation pressure on molecules may have a non-negligible influence on the dynamics and the driving of the wind even in the case of carbon-rich CDS. Therefore, already these investigations show that radiation pressure on molecules is an excellent candidate to initiate and to support the winds of oxygen-rich objects where dust formation alone might be too inefficient to maintain the outflow.

Although mean opacities are only a rough approximation for frequency-dependent opacities they are a very convenient tool to study the influence of radiation pressure on molecules on the dynamics of circumstellar outflows.

4. Influence of the grain opacity

The extinction properties of the dust component play a decisive role for the hydrodynamic and thermodynamic structure of a CDS and also determine its spectral appearance if relevant amounts of dust are formed.

In order to calculate these transport coefficients in the framework of Mie theory, the complex refractive index $m(\lambda)$ of the grain material has to be known.

However, the optical constants of the grains do not only depend on the dust material but also on the microscopic structure of the particles. In case of an ordered (crystalline) structure one finds a $1/\lambda^2$ - dependence of the FIR extinction, while a disordered (amorphous) structure gives a $1/\lambda$ - dependence. In the case of carbon dust, both structures, amorphous carbon and crystalline graphite, are possible.

The actual structure of the grains formed in the stellar wind is, of course, not known a priori but is a result of a complex interaction. Theoretical considerations predict the formation of inhomogeneous grains with crystalline cores surrounded by amorphous mantles (Gail & Sedlmayr 1984). Only the mantles interact with the radiation field, and hence, are accessible by observations.

Recent spectral modelling of observational results implies that the presence of amorphous grains rather than graphite is more likely in the circumstellar shells around C-stars (e.g. Griffin 1990; Orofino et al. 1990; Bagnulo et al. 1995).

Unfortunately, the optical properties of the grains, which decisively influence their physical environment, depend sensitively on their exact internal structure, e.g. the degree of crystallization and the hydrogen content, which in turn is sensitive to the physical conditions of their production.

Tables for the Planck–mean value of the dust opacity as a function of temperature were calculated from the data of the complex refractive index obtained in the laboratory. For details of the data we refer to the references given in Table 2. These tables were used in the dynamical model calculations and the resulting quantities (mass loss rates, terminal expansion velocities, dust-to-gas mass ratios) are given in Table 2.

It turns out that the mass loss rate and the dust-to-gas-ratio are unaffected by the table used to calculate the dust opacity. The opacity, however, directly determines the acceleration of the material, and hence, significantly influence the final outflow velocity. The overall structure of the outflow differs only slightly from the structure presented in Fig. 1.

Table 2. Resulting quantities of the evolved models for different data sets describing the complex refractive index of carbon grains. The parameters of the standard model are used.

table	$<\dot{M}>$ $[M_\odot \mathrm{yr}^{-1}]$	$<v_\infty>$ $[\mathrm{kms}^{-1}]$	$\rho_\mathrm{d}/\rho_\mathrm{g}$
AC1[1]	$1.1\,10^{-5}$	24.3	$4.2\,10^{-3}$
BE1[1]	$9.1\,10^{-6}$	32.5	$3.5\,10^{-3}$
HAPS[1]	$1.0\,10^{-5}$	33.1	$3.3\,10^{-3}$
FC21PS[1]	$1.1\,10^{-5}$	32.6	$3.5\,10^{-3}$
MARONAC[2]	$1.3\,10^{-5}$	27.8	$4.1\,10^{-3}$
POYHAC[3]	$1.0\,10^{-5}$	33.7	$4.0\,10^{-3}$
MWAC[4]	$9.4\,10^{-6}$	31.4	$3.6\,10^{-3}$
Graphite[5]	$1.2\,10^{-5}$	24.7	$4.1\,10^{-3}$

[1]: Rouleau & Martin (1991), [2]: Maron (1990), [3]: Preibisch et al. (1993), [4]: Mathis & Whiffen (1989), [5]: Draine (1985)

Although the dust opacity influences only marginally the dynamical behavior it has substantial influence on the optical appearance of the model, e.g. its position in a two-color diagram. This will be discussed in detail in a forthcoming paper (Winters & Fleischer 1998).

5. Concluding remarks

Dynamical models of carbon-rich outflows have reached a maturity in the last years which makes them ideal tools to interpret the observations. These models can still be improved; however, it is unlikely, that this will change the general picture we have now of these objects. Unfortunately, comparable studies of oxygen-rich outflows are not yet available, mainly because of the much more complex dust formation process in this case (see Jeong et al., in this volume)

Both, carbon-rich as well as oxygen-rich models are based on a simple approximation to simulate the interior pulsation. To combine dynamical atmospheric models with stellar pulsational models is one of the great challenges for stellar astrophysics in the next years.

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