Dynamical Opacity-Sampling Models of Mira Variables. II: 
Time-Dependent Atmospheric Structure and Observable Properties 
of 4 M-Type Model Series.

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ABSTRACT

We present 4 model series of the CODEX dynamical opacity-sampling models of Mira variables with solar abundances, designed to have parameters similar to o Cet, R Leo and R Cas. We demonstrate that the CODEX models provide a clear physical basis for the molecular shell scenario used to explain interferometric observations of Mira variables. We show that these models generally provide a good match to photometry and interferometry at wavelengths between the near-infrared and the radio, and make the model outputs publicly available. These model also demonstrate that, in order to match visible and infrared observations, the Fe-poor silicate grains that form within 3 continuum radii must have small grain radii and therefore can not drive the winds from O-rich Mira variables.

Key words: stars: AGB and post-AGB, stars: atmospheres, stars: variables: other, stars: mass loss

1 INTRODUCTION

Asymptotic Giant Branch (AGB) stars represent the final fusion-powered stage in the evolution of solar-type stars, and the engine by which the vast majority of the material in our Galaxy is recycled from stars back to the interstellar medium (Gall 2003). Mira variables represent the final stage in AGB evolution before they become dust-enshrouded and difficult to observe. They are so bright in the infrared that they can be used as competitive extragalactic distance indicators and probes of star formation history (Rejkuba 2003; Menzies et al. 2010). They are also unique amongst stellar classes in their opportunity for detailed observations: light curves that differ in shape and amplitude in different bandpasses, photospheres that show different sizes and structure as a function of wavelength, velocity-resolved motions and complex spectra.

The observational literature on Mira variables is very extensive, as partly detailed below in Section 3. In order to make sense of these observations, comprehensive models are required that link physical parameters to pulsation, and pulsation to observed properties and mass-loss. The previous generation of models (e.g. Hofner et al. 1998; Hofmann et al. 1998) suffered from grey or mean-opacity like approximations in their radiative transfer codes, so were not ideally suited to interpreting many observed properties, for example visible brightness or high-resolution spectroscopy. The next generation of models (Upsalla: Hofner et al. 2003, CODEX: Ireland et al. 2008) are better suited for modern observational comparisons, but extensive grids have not yet been produced, both because of solvable but difficult computational issues and the lack of a clear calibration for model parameters.

Here we present four physical model series for M-type Mira variables, as a first step in tuning and testing the CODEX models to derive physical parameters of Mira variables from observations, and to gain physical insight into the dominant physical processes in Mira-variable atmospheres. Observational predictions including predictions for infrared interferometry of the model series are made available online so that new observations can easily be compared to these models.

One of these model series has parameters based on o Cet, one based on R Leo and two are based on R Cas with different assumptions. For all models, only the pulsation period is guaranteed to match observations, and in this paper we aim to examine the other model outputs in order to more closely target model series to real stars in future papers. The model construction was described in Paper I (Ireland et al. 2008): they begin with input parameters of mass, luminosity and composition, with three other free parameters being set based on gravity, rotation and stellar wind. The model atmospheres are then constructed by solving the hydrostatic structure equations, and the pulsation is self-excited (i.e. it occurs spontaneously), and the temperature of all layers is calculated by solving the energy equation.

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the conservation of energy equation via a detailed opacity-sampling method.

Details of the parameter choices for the model series are given in Section 2 as well as basic comparison of the model light curves to observations. Model predictions for spectra, in particular the effect of extension on spectra, are tested in Section 3 and the models are compared to observations of ζ Cet including infrared and radio interferometry in Section 4. In Section 5 we compare the model structures to previously published ad-hoc molecular shell papers, and in Section 6 we discuss the mass loss rates of the models and the driving mechanisms. In Section 7 we discuss the effect of input parameters on the models, and the possibility for better calibrating the input parameters so that, e.g. the mass of individual Miras could be inferred from models. Finally, in Section 8 we conclude and discuss plans for future work.

2 MODEL PARAMETERS AND DESCRIPTION

A detailed description of the model construction was given in Paper I. Briefly, the models consist of self-excited grey models that determine the atmospheric pressure stratification and luminosity. The temperature profile is then re-iterated using an opacity sampling code with 4300 wavelength points, assuming radiative and local thermodynamic equilibrium. Dust formation follows Ireland & Scholz (2006), except that we drop the Rayleigh approximation, instead replacing it by a smooth fit to the Mie approximation of spherical grains, weighting the Rayleigh scattering by:

\[ \sigma_M(a, \lambda) = \sigma_R(a, \lambda)(1 + 4.5\frac{a}{\lambda})^{-1}, \]

where \(a\) is the grain radius, \(\lambda\) the wavelength of radiation, \(\sigma\) the scattering cross-section and \(\sigma_R\) the scattering cross-section in the Rayleigh approximation. This cross-section \(\sigma_M\) is the total cross-section weighted by \((1-\mu)\), where \(\mu\) is the impact parameter. This weighting ensures that the radiative acceleration on dust is correct in the presence of forward-scattering.

The choice of free parameters was only briefly discussed in Paper I in the context of the ο54 model series, based on the parameters of the prototype Mira variable ο Cet. The input parameters for all 4 model series presented here are given in Table 1 and the reasons for their choice give in sub-sections below.

The behavior over \(10^4\) days of each nonlinear pulsation model series is shown in Figures 1–4. As each model series runs for many cycles, we chose only a few representative models were extracted and their velocity and pressure structures used as input to the model atmosphere code which, after temperature iteration, give spectra and centre-to-limb variation (CLV) for the models. The cycles during which models were extracted are shown as shaded regions in Figures 1–4 and the actual models extracted are shown as circles in the top panels of these figures. The instantaneous physical parameters and shock front locations for the chosen models are given in Tables 4–8 (available in their entirety in the on-line version of the journal). We note that the model radius is defined in these tables as the radius where the Rosseland optical depth is unity, and the effective temperature is defined by this radius.

For all 4 model series, we assume solar element abundances from Grevesse et al. (1996). This is near the mean abundance observed for stars in the solar vicinity with ages of 3–6×10^9 years (Edvardsson et al. 1993). Our red giant model with mass 1.35 M_☉ has an age of ~3×10^9 years and the red giant model with mass 1.1 M_☉ has an age of ~6×10^9 years according the isochrones of Girardi et al. (2000). However, as shown by Edvardsson et al. (1993), there is a scatter in [Fe/H] from about -0.5 to +0.3 for stars of this age, so that the Mira stars we are aiming to model could have somewhat different abundances to those we have adopted.

The adopted value for the mixing length in units of pressure-scale height for the ο54, R52 and C81 series, \(\alpha_m\), and turbulent viscosity parameter \(\nu_p\) are input parameters, and the parent-star radius \(R_p\) and period \(P\) are derived parameters.

| Name | M (M_☉) | L (L_☉) | Z | \(\alpha_m\) | \(\nu_p\) | \(R_p\) (R_☉) | \(P\) (days) | \(P_{\text{linear}}\) |
|------|---------|---------|---|-------------|---------|--------------|----------|----------|
| ο54  | 1.1     | 5400    | 0.02 | 3.5         | 0.25    | 216          | 330      | 261      |
| R52  | 1.1     | 5200    | 0.02 | 3.5         | 0.25    | 209          | 307      | 243      |
| C50  | 1.35    | 5050    | 0.02 | 2.0         | 0.24    | 291          | 427      | 408      |
| C81  | 1.35    | 8160    | 0.02 | 3.5         | 0.32    | 278          | 430      | 374      |

Figure 1. The luminosity (top panel), effective temperature (middle panel), and the radii of a representative selection of mass zones (bottom panel) plotted against time for model ο54. The red line in the bottom panel shows the position of the point where the grey approximation optical depth \(\tau_g = 2/3\), \(T_{\text{eff}}\) in the middle panel is here defined as the temperature where \(\tau_g = 2/3\), which is close to the effective temperature \(\propto (L/R^2)^{1/4}\) of the non-grey atmospheric stratification. The shaded regions show the time intervals in which models were selected for detailed atmospheric model computation. The selected models are circled in the top panel. The mass, luminosity, metallicity and period of the nonlinear pulsation model are shown at the top of the plot.
outer convective layers, causing the model star to expand. Therefore mixing length has been used by us as a way to produce the correct period, given a luminosity $L$. However, this procedure is always ambiguous for a given field Mira, because the distance and hence $M$ is always uncertain by $\sim 10\%$ or more. The value of $\alpha_\nu$ can be adjusted to give the correct pulsation amplitude. Alternatively, within limits, $M$ can adjusted to give the correct pulsation amplitude. Thus far in our models series, we have assumed values of $M$ based on e.g. typical masses as a function of period and then used $\alpha_\nu$ to tune the pulsation amplitude. By comparing these model series with observations, we aim to develop a preferred values for $\alpha_m$ and $\alpha_\nu$, or at least a preferred prescription for choosing $\alpha_m$ and $\alpha_\nu$ as a function of the physical input parameters $M$, $L$ (a proxy for evolutionary state along the AGB) and $Z$.

Although our models have been generally based on the stars o Cet, R Leo and R Cas, there are a range of parameters that are consistent with these Miras, and a detailed comparison with observations will inevitably reveal where the differences lie. In the following section, we aim to discuss the chosen parameters for each model series, compare predicted light curves to observed light curves and draw preliminary conclusions as to whether changes to physical input parameters could improve model fits. We choose the $V$, $J$ and $K$ band for comparison to observations: $V$ band because of the wealth of observational data, and $J$ and $K$ because the model predictions are most reliable in these band-passes. For this comparison, we add 0.5 magnitudes to the predicted $V$-band fluxes, to account for non-LTE effects as computed in the models at selected phases in Paper I, where the correction needed varies between 0.3 and 1.0 magnitudes.

2.1 o54 5400 $L_\odot$ series

The 5400 $L_\odot$ model series for o Cet ($P = 332$ days) has model parameters chosen to match the luminosity obtained from the $J$ and $K$ photometry of Whitelock et al. (2000) and the Knapp et al. (2003) revised HIPPARCOS parallax. The mass of 1.1 $M_\odot$ was adopted since an analysis of the Galactic scale height of Mira variables by Jura & Kleinmann (1992) suggest a mass of $\sim 1.1$ $M_\odot$ for Mira variables with periods from 300–400 days, while a study of the population of Miras by Wyatt and Cahn (1983) gives a progenitores of 4 $M_\text{type}$ Model series

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ior mass estimate of 1.18 \( M_\odot \) for \( \sigma \) Cet. We give this model series the designation \( \sigma 54 \).

Figure 5 shows the light curves derived from 4 cycles of the \( \sigma 54 \) model series between times 8000 and 10\(^3\) days in Figure[1][1]. To fit the K-band maximum flux, \( \sigma \) Cet needs to be at a distance of 107 pc. This corresponds to a parallax of 9.1 mas, consistent with the van Leeuwen (2007) value of 10.91\( \pm \)1.22 mas from HIPPARCOS.

The models fit the general light-curve shape and amplitude, but they are \(-0.1\) magnitudes too blue in \( J-K \) colour, too blue in \( V-K \) by \(-1\) magnitudes (hence too bright in \( V \) near maximum by \(-1\) magnitudes), and these 4 cycles do not reproduce the cycle-to-cycle scatter in \( J \) and \( K \) magnitudes near minimum.

We also computed models for more compact atmosphere cycles (between times 1000 and 2000 days in Figure 1) and more extended atmosphere cycles (between times 3500 and 4300 days), but \( J \), \( H \) and \( V \) fluxes were not noticeably different. The atmospheric structures for the various models are shown in Figure[1][1]. The consistently blue \( J-K \) and \( V-K \) colours suggest that \( T_{\text{eff}} \) is too high in the model (see Section 5 for more discussion).

Although the basic model properties \( (L, R, T_{\text{eff}}) \) and the near-continuum fluxes are similar from cycle to cycle, high-layer observational features differ depending on the upper atmosphere structure. The reason for this can be seen in Tables[2][2]through[7][7], where upper layer shock front positions are not repeatable from cycle to cycle. For example, in Table[2][2] at phase -0.2, the upper strong shock from a previous cycle is at 2.82 \( R_\odot \). Exactly 1 cycle later, at phase 0.8, the upper shock has just merged with a lower shock at 1.82 \( R_\odot \).

### 2.2 \( R52 \ 5200 \ L_\odot \) series

The period of \( R \) Leo is slightly shorter than that of \( \sigma \) Cet, and we chose to model \( R \) Leo with a model identical to the \( \sigma \) Cet model, but with a luminosity reduced to match the smaller period (310 versus 332 days). Miras typically also have reduced masses at reduced periods (Jura & Kleinmann 1992), but we chose not to reduce the mass so as to see the differential influence of luminosity alone (Wyatt and Cahn 1983 give a mass of 1.04 \( M_\odot \) for \( R \) Leo). The model has a luminosity derived by assuming \( R \) Leo was at a distance of 110 pc, corresponding to a parallax of 9.1 mas, again consistent with the van Leeuwen (2007) value of 14.03\( \pm \)2.65 mas within 2\( \sigma \).
Table 5. Parameters of the extended 2 cycles of the R52 series, including the position of the shock fronts. [To be available online only]

| Model  | Phase | L  | R  | T_eff | S1 | S2 | S3 | S4 |
|--------|-------|----|----|-------|----|----|----|----|
|        |       | ($L_\odot$) | ($R_p$) | (K) | ($R_p$) | ($R_p$) | ($R_p$) | ($R_p$) |
| 360540 | -0.20 | 4442 | 0.92 | 3411 | 2.02 | 0.93 |
| 360760 | -0.10 | 5000 | 0.91 | 3535 | 1.94 | 0.92 |
| 361180 | 0.00  | 8266 | 1.06 | 3696 | 1.79 | 1.11 |
| 361720 | 0.10  | 7425 | 1.24 | 3338 | 1.57 | 1.40 |
| 361860 | 0.19  | 6491 | 1.33 | 3118 | 1.71 |       |
| 361900 | 0.32  | 4700 | 1.36 | 2844 | 2.10 |       |
| 361920 | 0.46  | 3729 | 1.25 | 2793 | 2.38 |       |
| 361940 | 0.54  | 2795 | 1.15 | 2714 | 2.51 |       |
| 362020 | 0.60  | 2901 | 1.06 | 2851 | 2.58 | 1.06 |
| 362200 | 0.70  | 3837 | 0.96 | 3209 | 2.69 | 0.97 |
| 362380 | 0.80  | 4405 | 0.92 | 3400 | 2.79 | 0.94 |
| 362560 | 0.90  | 5083 | 0.91 | 3545 | 2.81 | 0.92 |
| 362780 | 1.00  | 8236 | 0.99 | 3209 | 2.87 | 1.10 |
| 363000 | 1.10  | 7408 | 1.24 | 3337 | 2.93 | 1.37 |
| 363180 | 1.20  | 6374 | 1.33 | 3097 | 2.89 | 1.59 |
| 363380 | 1.30  | 4897 | 1.36 | 2870 | 2.92 | 1.77 |
| 363540 | 1.41  | 4088 | 1.31 | 2797 | 2.81 | 1.91 |
| 363600 | 1.49  | 3063 | 1.24 | 2674 | 1.97 |       |
| 363700 | 1.60  | 2567 | 1.06 | 2767 | 2.00 | 1.05 |
| 363900 | 1.70  | 3910 | 0.96 | 3225 | 2.00 | 0.97 |
| 364120 | 1.80  | 4456 | 0.93 | 3332 | 2.18 |       |
| 364380 | 1.90  | 5076 | 0.91 | 3544 | 2.18 | 0.93 |
| 364960 | 2.00  | 8304 | 1.07 | 3699 | 1.76 | 1.12 |

Table 6. Parameters of the compact 2 cycles of the R52 series, including the position of the shock fronts. [To be available on-line only]

| Model  | Phase | L  | R  | T_eff | S1 | S2 | S3 | S4 |
|--------|-------|----|----|-------|----|----|----|----|
|        |       | ($L_\odot$) | ($R_p$) | (K) | ($R_p$) | ($R_p$) | ($R_p$) | ($R_p$) |
| 386200 | 2.36  | 4640 | 1.35 | 2836 | 2.18 |       |
| 386280 | 2.49  | 3813 | 1.26 | 2796 | 2.56 |       |
| 386320 | 2.60  | 2569 | 1.13 | 2680 | 2.89 | 1.10 |
| 386500 | 2.70  | 3753 | 0.99 | 3148 | 3.09 | 1.00 |
| 386660 | 2.80  | 4198 | 0.93 | 3332 | 3.27 | 0.95 |
| 386840 | 2.90  | 4680 | 0.90 | 3486 | 3.46 | 0.92 |
| 387040 | 3.00  | 8026 | 0.99 | 3801 | 1.02 |       |
| 387260 | 3.10  | 7704 | 1.18 | 3446 | 1.27 |       |
| 387420 | 3.19  | 6844 | 1.30 | 3193 | 1.49 |       |
| 387580 | 3.30  | 5449 | 1.36 | 2951 | 1.70 |       |
| 387700 | 3.40  | 4350 | 1.34 | 2805 | 1.85 |       |
| 387780 | 3.49  | 3585 | 1.27 | 2743 | 1.93 |       |
| 387860 | 3.61  | 2049 | 1.24 | 2421 | 1.98 | 1.09 |
| 388040 | 3.70  | 3560 | 0.99 | 3111 | 1.97 | 0.99 |
| 388240 | 3.80  | 4311 | 0.93 | 3355 | 1.92 | 0.95 |
| 388480 | 3.90  | 4704 | 0.90 | 3483 | 1.83 | 0.93 |
| 388900 | 4.00  | 8166 | 0.99 | 3814 | 1.69 | 1.03 |
| 389540 | 4.10  | 7818 | 1.17 | 3473 | 1.48 | 1.30 |
| 389680 | 4.20  | 6744 | 1.31 | 3172 | 1.69 |       |
| 389720 | 4.32  | 5120 | 1.35 | 2908 | 2.06 |       |
| 389740 | 4.49  | 3819 | 1.26 | 2803 | 2.45 |       |
| 389780 | 4.60  | 2700 | 1.12 | 2728 | 2.65 | 1.10 |
| 389940 | 4.69  | 3700 | 0.99 | 3128 | 2.77 | 1.00 |
| 390120 | 4.80  | 4182 | 0.93 | 3332 | 2.88 | 0.95 |
| 390300 | 4.90  | 4674 | 0.90 | 3482 | 3.01 | 0.93 |

It is clear in Figure 6 that this model is too blue to be an effective model for R Leo in both $V-K$ and $J-K$ colours, and has a visual amplitude much larger and a $K$ amplitude slightly larger than R Leo. The amplitude of the R Leo model is slightly smaller than the amplitude of the o Cet model due to the reduced luminosity. This luminosity change by itself is not enough to explain the different visual amplitudes of the real R Leo and o Cet. It is possible that these two stars have different metallicity (i.e. the redder colours of R Leo could be because it has a higher metallicity). A difference in mass is also possible, with a compensating change in luminosity within that allowed by the parallax error to retain the same period.

Like the o54 series, we computed an extended sub-series (day numbers 3600–4500 in Figure 2) and a compact sub-series (day numbers 3600–4500 in Figure 2).
numbers 8200–9100 in Figure 2. The compact sub-series had its detailed radiative transfer model truncated at 4 \( R_p \), because the very low density in the outer layers (< 10^{-15} \text{ g cm}^{-3} ) had extremely low opacity and the models had outer-layer physical conditions outside the range where our equation of state was valid. Again, the \( V \), \( J \) and \( K \) fluxes were similar in each case (only the extended sub-series is displayed).

Table 7. Parameters of the \( C50 \) series, including the position of the shock fronts.[To be available on-line only]

| Model     | Phase | \( L (L_{\odot}) \) | \( R (R_{\odot}) \) | \( T_{\text{eff}} \) (K) | S1 \( (R_p) \) | S2 \( (R_p) \) | S3 \( (R_p) \) | S4 \( (R_p) \) | S5 \( (R_p) \) |
|-----------|-------|---------------------|---------------------|---------------------|--------------|--------------|--------------|--------------|--------------|
| 375360    | -1.30 | 2673                | 0.92                | 2532                | 2.49         | 0.92         |              |              |              |
| 375490    | -1.20 | 3407                | 0.85                | 2810                | 2.56         | 0.87         |              |              |              |
| 375630    | -1.10 | 3529                | 0.80                | 2924                | 2.59         | 0.83         |              |              |              |
| 375780    | -1.00 | 6640                | 0.87                | 3271                | 2.63         | 0.92         |              |              |              |
| 375920    | -0.90 | 7218                | 1.03                | 3077                | 2.62         | 1.13         |              |              |              |
| 376050    | -0.80 | 7039                | 1.16                | 2883                | 2.60         | 1.37         |              |              |              |
| 376160    | -0.70 | 6412                | 1.23                | 2738                | 2.55         | 1.57         |              |              |              |
| 376260    | -0.60 | 5537                | 1.24                | 2627                | 2.48         | 1.74         |              |              |              |
| 376330    | -0.50 | 4263                | 1.21                | 2493                | 2.38         | 1.84         |              |              |              |
| 376380    | -0.40 | 2851                | 1.10                | 2357                | 2.19         | 1.91         |              |              |              |
| 376470    | -0.30 | 2678                | 0.92                | 2543                | 1.93         | 0.92         |              |              |              |
| 376630    | -0.20 | 3392                | 0.84                | 2816                | 1.97         | 0.87         |              |              |              |
| 376820    | -0.10 | 3595                | 0.80                | 2937                | 1.97         | 0.82         |              |              |              |
| 377110    | 0.00  | 6722                | 0.88                | 3261                | 1.86         | 0.94         |              |              |              |
| 377490    | 0.10  | 7253                | 1.04                | 3058                | 1.75         | 1.18         |              |              |              |
| 377710    | 0.20  | 7037                | 1.16                | 2876                | 1.53         |              |              |              |              |
| 377750    | 0.30  | 6400                | 1.23                | 2735                | 2.01         |              |              |              |              |
| 377760    | 0.40  | 5465                | 1.24                | 2618                | 2.39         |              |              |              |              |
| 378020    | 0.53  | 3720                | 1.21                | 2407                | 2.83         |              |              |              |              |
| 377790    | 0.61  | 2633                | 1.18                | 2233                | 3.06         |              |              |              |              |
| 377880    | 0.70  | 2883                | 0.91                | 2606                | 3.31         | 0.91         |              |              |              |
| 378020    | 0.80  | 3370                | 0.84                | 2823                | 3.55         | 0.86         |              |              |              |
| 378160    | 0.90  | 3813                | 0.80                | 2981                | 3.76         | 0.82         |              |              |              |
| 378320    | 1.00  | 6750                | 0.89                | 3253                | 3.96         | 0.93         |              |              |              |
| 378470    | 1.10  | 7246                | 1.06                | 3035                | 4.15         | 1.18         |              |              |              |
| 378570    | 1.21  | 6955                | 1.18                | 2852                | 4.34         | 1.44         |              |              |              |
| 378630    | 1.31  | 6250                | 1.23                | 2713                | 4.52         | 1.65         |              |              |              |
| 378660    | 1.40  | 5395                | 1.24                | 2610                | (4.66)       | 1.80         |              |              |              |
| 378680    | 1.49  | 4166                | 1.21                | 2476                | (4.80)       | 1.91         |              |              |              |
| 378710    | 1.61  | 2512                | 1.06                | 2326                | (4.97)       | 1.97         |              |              |              |
| 378810    | 1.70  | 2972                | 0.90                | 2631                | 1.95         | 0.91         |              |              |              |
| 378960    | 1.80  | 3380                | 0.83                | 2827                | 1.89         | 0.86         |              |              |              |

2.3 \( CB1 \ 8160 \ L_{\odot} \) series

With the same input physics as the \( o \) Cet models, we attempted to create a longer period series appropriate for the Mira variable R Cas (\( P = 430 \) days) by increasing the luminosity and mass. However, the model pulsation amplitude became much too large, requiring us to increase the \( \alpha_L \) parameter. The HIPPARCOS distance for R Cas in Whitelock et al. (2008) would require the star to be very underluminous when compared with the mean solar-vicinity P-L relationship of Whitelock et al. (2008) or the LMC P-L relationship (e.g Hughes & Wood 1990). For this model series, the luminosity of our model was derived by assuming R Cas falls on the mean solar-vicinity P-L relationship of Whitelock et al. (2008) and is at a distance of 204 pc, with a corresponding parallax of 4.9 mas, almost 3-\( \sigma \) from the \( \text{van Leeuwen} \) (2007) value of 7.95 ± 1.02 mas. The mass adopted for R Cas is 1.35 \( M_{\odot} \) as given by Wyatt & Cahn (1983).

The light curves of R Cas in the \( V \), \( J \) and \( K \) bands are shown in Figure 8 corresponding to day numbers ~4000-5700 chosen for detailed radiative transfer computation in Figure 3. The \( J \) and \( K \) light curves of the model fit the observations quite well, while in all cycles where the near-maximum model was computed, the models are too bright in \( V \) near maximum light. The near-maximum continuum effective temperature is ~3800 K in Table 8 corresponds to an M0 or M1 giant according to the temperature calibration of Fluks et al. (1994) and appears like an M2 giant in the TiO features as predicted by our model spectra. This is much too warm for
Table 8. Parameters of the C81 series, including the position of the shock fronts. [To be available on-line only]

| Model | Phase | L (L⊙) | R (Rp) | T eff (K) | S1 (Rp) | S2 (Rp) | S3 (Rp) | S4 (Rp) | S5 (Rp) | S6 (Rp) |
|-------|-------|--------|--------|----------|---------|---------|---------|---------|---------|---------|
| 243570 | -0.40 | 3917 | 1.58 | 2182 | 2.74 | 1.96 |
| 243670 | -0.30 | 3705 | 1.34 | 2336 | 2.40 | 2.06 | 0.98 |
| 244000 | -0.20 | 5772 | 0.87 | 3235 | 2.14 | 2.07 | 0.87 |
| 244140 | -0.10 | 5133 | 0.79 | 3311 | 2.29 | 2.07 | 0.81 |
| 244330 | 0.00 | 9462 | 0.81 | 3811 | 2.25 | 2.07 | 0.81 |
| 244700 | 0.10 | 12120 | 1.28 | 3212 | 2.20 | 1.94 |
| 244810 | 0.20 | 11150 | 1.40 | 3015 | 2.05 | 1.87 |
| 244910 | 0.30 | 8327 | 1.44 | 2758 | 2.31 |
| 244940 | 0.52 | 5324 | 1.65 | 2310 | 2.82 |
| 244960 | 0.61 | 4427 | 1.84 | 2087 | 3.07 |
| 247020 | 0.10 | 5772 | 0.87 | 3235 | 2.14 | 0.87 |
| 247140 | 0.20 | 5133 | 0.79 | 3311 | 2.29 | 0.79 |
| 247330 | 0.30 | 9462 | 0.81 | 3811 | 2.25 | 0.81 |
| 247500 | 0.50 | 12120 | 1.28 | 3212 | 2.20 | 1.49 |
| 247580 | 0.60 | 11150 | 1.40 | 3015 | 2.05 | 1.87 |
| 247690 | 0.70 | 8327 | 1.44 | 2758 | 2.31 |
| 247810 | 0.80 | 5324 | 1.65 | 2310 | 2.82 |
| 247900 | 0.90 | 4427 | 1.84 | 2087 | 3.07 |
| 247970 | 1.00 | 3972 | 1.58 | 3015 | 2.05 | 1.87 |
| 248020 | 1.10 | 12120 | 1.28 | 3212 | 2.20 | 1.49 |
| 248130 | 1.20 | 11150 | 1.40 | 3015 | 2.05 | 1.87 |
| 248280 | 1.30 | 8327 | 1.44 | 2758 | 2.31 |
| 248350 | 1.40 | 5324 | 1.65 | 2310 | 2.82 |
| 248430 | 1.50 | 4427 | 1.84 | 2087 | 3.07 |
| 248580 | 1.60 | 3972 | 1.58 | 3015 | 2.05 | 1.87 |
| 248730 | 1.70 | 12120 | 1.28 | 3212 | 2.20 | 1.49 |
| 248870 | 1.80 | 11150 | 1.40 | 3015 | 2.05 | 1.87 |
| 248900 | 1.90 | 8327 | 1.44 | 2758 | 2.31 |
| 249020 | 2.00 | 5324 | 1.65 | 2310 | 2.82 |

R Cas which has a catalogued spectral type of M6–M10. Therefore, we are forced to conclude that $T_{\text{eff}}$ is too high for this model.

2.4 C50 5050 L⊙ series

As the 8160 L⊙ model or R Cas was so clearly discrepant near maximum, and as the individual HIPPARCOS distance in Whitelocket et al. (2008) would give a luminosity of only $\sim 3770 L_\odot$, we chose to construct a lower luminosity model. The luminosity was determined by fixing the mixing length parameter which was decreased to a more standard value of $\alpha_m = 2$. The luminosity was then tuned to match the model period to that of R Cas. As usual, the turbulent viscosity parameter was then tuned to match the bolometric amplitude of R Cas and the model. The resulting luminosity (5050 L⊙) suggests that R Cas is at a distance of 166 pc with a corresponding parallax of 6.0 mas: this is now consistent with the HIPPARCOS value within 2-σ.

The near-maximum effective temperature of this model is now $\sim 3250 K$, both consistent with an M6 spectral type from the calibration of Fluks et al. (1994) and providing a better match to the observed M6 spectra in Fluks et al. (1994) than either M5 of M7 spectra. It also has a a $V-K$ colour that matches that of R Cas (see Figure 7).

2.5 Using the Models

For each model phase in Tables 3 through 8 we provide the full model output. Indeed, this output was already used by Woodruff et al. (2009) in advance of publication in order to compare the models to wavelength-dispersed infrared interferometry. A sample 3 lines from one of these tables is given in Table 9. In order to use these models to compare to a specific observation, integration over a filter profile $F(\lambda)$ is required:

$$L_F = \int L(\lambda) d\lambda$$ (2)
Table 9. An excerpt of the table available on-line describing the model output for the o54 series model 285180. The center-to-limb variation (CLV) is shown as a fraction of the central intensity $I_0$ as a function of normalized radius on the apparent stellar disk, $r/5R_p$.

| Wavelength ($\mu m$) | $L_\lambda$ (erg s $\mu m^{-1}$) | $I_0$ (erg s cm$^{-2}$ $\mu m^{-1}$ sr$^{-1}$) | CLV: $r/5R_p$ | $I/I_0$ |
|---------------------|-----------------------------------|-----------------------------------------------|----------------|---------|
|                     |                                   |                                               | 0.020          |         |
| 1.598               | 0.9786E+37                       | 0.1124E+10                                   | 0.997          |         |
| 1.599               | 0.8160E+37                       | 0.3054E+09                                   | 0.999          |         |
| 1.600               | 0.1106E+38                       | 0.1427E+10                                   | 0.998          |         |

Figure 4. The luminosity and mass-zone positions in the C50 series, showing the locations of the phases chosen for detailed model computation.

Figure 5. Light curves of the o54 series in $J$, $K$ and $V$ bands compared with observations of o Cet by Whitelock et al. (2000) and the AFOEV.

Figure 6. Light curves of the R52 series in the extended cycle in $J$, $K$ and $V$ bands compared with observations by Whitelock et al. (2000) and the AFOEV.

Figure 7. Light curves of the C50 series $J$, $K$ and $V$ bands compared with observations by Nadzhip et al. (2001) and the AFOEV.

Figure 8. Light curves of the C81 series $J$, $K$ and $V$ bands compared with observations by Nadzhip et al. (2001) and the AFOEV.
3 MODEL SPECTRA

The spectra computed in the CODEX models using the default wavelength table come from an opacity sampling method with a spectral resolution of up to $\sim 10^5$. However, in order to accurately compare with observations at any wavelength, at least $\sim 100$ wavelengths have to be averaged together, preferably using a non-square edged filter. In turn, this means that these default model outputs can only be used at a spectral resolution of $R \sim 100$ or lower. This is especially true where the CO bands in $H$ and $K$ bands are concerned, where there is a combination of very strong absorption and near-continuum spectral features.

For the purposes of comparing spectra with observations in $H$- and $K$-bands, we therefore also computed spectra and center-to-limb variations at $R \approx 10^5$ in these bands. In Figures 9 and 10 we convolved the model spectra with a Gaussian of Full-Width Half Maximum equivalent to a spectral resolution of $R = 1000$, and compared the model spectra with observations of the Mira variable R Cha from Lancón & Wood (2000). We chose to compare with the o54 series, because the parameters of R Cha are most like those of o Cet. There was an arbitrary scaling applied to the observed spectra. These factors differed by 0.05 mags between the $H$- and $K$-bands for the phase 0.1 spectrum and 0.15 magnitudes for the phase 0.3 spectrum: these small differences. The best model fits were from phases 0.3 and 0.6, where temperatures were $\sim 500$ K cooler than phases applicable to the R Cha observations. This demonstrates that in the CO overtone bands, the models are too hot for R Cha. To make this statement more quantitatively based on spectral synthesis, metallicity effects would have to be considered also (beyond the scope of this paper).

\[ I_F(x) = \int \frac{F(\lambda)}{I_0(\lambda)} f(x, \lambda) d\lambda. \] (3)

Here $L_F$ is the stellar luminosity as seen through the filter, $I_F(x)$ is the intensity profile seen through the filter, $I_0(\lambda)$ are the tabulated values of the central intensity and $f(x, \lambda)$ are the tabulated values of the normalized CLVs. It is much more preferable to use realistic filter profiles $F(\lambda)$ with smooth edges (e.g. a Gaussian) rather than square-edged filters in order to minimise noise due to the opacity sampling. Interferometric visibilities can then be obtained from the Hankel transform of $I_F(x)$.

4 OBSERVATION AND MODEL COMPARISON: O CET

The grand total of all available observations for Mira variables with parameters similar to those of the model series presented here is far too vast to compare to the model series of this paper in a concise manner. Therefore, we have chosen to examine the available observations of o Cet in a general sense to describe the similarities and differences between the o54 series and o Cet to further illustrate the utility of the model series and the wealth of information available to constrain models.

Table 10 summarizes most of the key observations available for o Cet. Time-dependent photometry is available between ultraviolet and radio wavelengths, with the best light curves available in the $V$, $J$, $H$ and $K$ bands, as shown in Figure 5 (V, J, K). There is reasonable agreement between the model and observations for light curve shape, amplitude and visible-infrared phase offsets.

Spectral classification should also give an observed effective temperature. Unfortunately, the MK spectral classification (e.g. Keenan et al. 1974) is based on B and V bands, where non-LTE effects in an extended atmosphere are very strong (Ireland et al. 2008). Consequently, the combination of effective temperature and metallicity can not be directly fit to observations. Spectra of o Cet are also not available electronically to the knowledge of the authors – a modern library of bright Mira spectra would certainly be of great use to future modelling efforts. In particular, infrared spectra are a much more reliable model output, and phase-dependent infrared spectra would be a wonderful tool for tuning model parameters.

Resolved observations have been made at wavelengths between 346 nm and 7 mm, with the broad range of highly wavelength dependent diameters being consistent with Models. The form of an angular diameter versus wavelength curve as shown in Woodruff et al. (2009) between 1 and 4 microns was very similar to the o54 model series, however, in that paper, the models were placed at a distance that best fit the angular diameters. If instead the models are placed at the distance that best fits the K-band photometry, the angular diameters as a function of phase are given in Figures 11 to 13. It is clear that the mean diameter of the models are too small, and that the phase-dependence of the observed diameter is less pronounced than in the model. Possible solutions to this are given in Sections 5 and 7.

In the radio, the measured angular size of o Cet corresponds to the angular size of the Na and/or $K$ ionisation edges. The consistency between models and observations shows that local thermal equilibrium is a reasonably assumption for defining the ionization
Figure 11. Model diameters of the α54 series in a narrow 1.24 μm band-pass based on fitting to a single spatial frequency where $V = 0.6$, with the measured diameters from Woodruff et al. (2008) over-plotted.

Figure 12. The same as Figure 11 except for the H-band.

Figure 13. The same as Figure 11 except for the K-band.

5 PREDICTING FUNDAMENTAL PARAMETERS WITH MODELS AND OBSERVATIONS

For each Mira variable modeled in this paper, there are currently 3 physical ($M$, $L$ and $Z$) parameters and 2 model parameters ($\alpha_m$ and $\alpha_\nu$). In the parameter neighborhood of the α54 series, we find that the radius of the “parent” star approximated by linear pulsation is given by:

$$R_* \approx \left( \frac{L_*}{5400L_\odot} \right)^{0.8} \left( \frac{M_*}{1.1M_\odot} \right)^{-0.4} \left( \frac{\alpha_m}{3.5} \right)^{0.7} \left( \frac{Z}{0.02} \right)^{0.2},$$

or in angular units:

$$\theta_* \propto d \left( \frac{F_*}{L_*} \right)^{0.8} \left( \frac{M_*}{\alpha_m} \right)^{-0.4} \left( \frac{Z}{0.02} \right)^{0.2},$$

where $d$ is the distance, and $F$ is the received wavelength-integrated stellar flux. In this section we will only discuss the most direct measurements of effective temperature, derived from near-continuum interferometry and photometry, as spectral fitting in the presence of non-LTE effects (Ireland et al. 2008), metallicity and abundance errors has yet to be demonstrated for extended M giants.

There is no dependence of the radius on $\alpha_\nu$, but there is a small dependence of the period $P$ on $\alpha_\nu$ which we will neglect here. The period, which typically is expressed in terms of mass and radius (the so-called PMR relationship), we will express in terms of our model parameters $L_\star$, $M_\star$, and $\alpha_m$:

$$P \approx \frac{261d}{L_\star} \left( \frac{L_*}{5400L_\odot} \right)^{1.8} \left( \frac{M_*}{1.1M_\odot} \right)^{-1.8} \left( \frac{\alpha_m}{3.5} \right)^{-1.5} \left( \frac{Z}{0.02} \right)^{0.4}.$$

Although these relationships are only approximate and do not hold over a wide range of parameters, they demonstrate the complex interplay between the model input parameters. In principle, a measurement of $Z$ from spectral synthesis, and measurements of period, amplitude, angular diameter, luminosity and distance are enough to constrain $M$, $\alpha_m$, and $\alpha_\nu$. However, a 10% distance uncertainty (the best of any nearby Mira) translates into a 20% $L$ uncertainty, or a 20% mass uncertainty keeping everything else fixed at a given period. The relationships are further complicated by the non-linear pulsation period differing significantly from the linear pulsation period (e.g. Table 1), depending on amplitude.

Consider first the problem of calibrating mass independently of pulsation models. Orbital periods for non-interacting Miras are far too long for combined visual and spectroscopic combined orbits to obtain dynamical masses due to the large radii of Miras. Clusters form a potential hunting ground for Mira variables where the AGB can be calibrated at a known initial mass (e.g. Lebzelter & Wood 2007), but the final mass of the Mira is a function of the assumed mass loss history, clusters do not easily provide the same age and metallicity range of Miras as in the field, and a direct radius measurement is not yet possible. Mass can also be estimated from kinematics. This is best done for Miras with kinematics inconsistent with the thick disk or halo. The best example of this for nearby Miras is o Cet.

o Cet has a ($U,V,W$) space velocity of (-26, -62, -89) km s$^{-1}$ when using the revised HIPPARCOS distance from van Leeuwen (2007). This space velocity is unusually large for a Mira, which is a major reason why the interaction between o Cet and the interstellar medium produces such an impressive tail (Martin et al. 2007). Although kinematics is often inconclusive when applied to individual stars, this space velocity falls within the 97% probability contour for thick disk membership according to Reddy et al. (2006). In the detailed analysis of Robin et al. (2003), the W velocity of o Cet is inconsistent at 5σ with even the old (5-10 Gyr) thin disk, and is most consistent with being a member of the thick disk, modeled as a single stellar population of 11 Gyr age. Importantly, o Cet can not be a runaway star (e.g. Hoogerwerf et al. 2000) where its space velocity is due to a single strong gravitational interaction in its past, because it has retained its wide companion Mira B, and the orbit
can not be highly eccentric as the periastron must be outside the at-
certainly less than 1.1
ary tracks places a 1.06 M
spectral fitting for R Cha, and the measured angular diameters.
and the mass of 1.35
less for sub-solar metallicity). This places the current mass of
pieces of evidence: the near-maximum
maturity, colour), except for its more uncertain distance. In Section 3,
was that the models were ~500 K too hot for R Cha. However, R Cha has the hottest near-maximum spectral type of all Mira variables at periods of ~300–350 days in Keenan et al. (1974), so this suggests that the models are too hot for any Mira. Inspection of some low-metallicity test models (to be published) indicates that decreasing the metallicity reduces this discrepancy but does not remove it.

Although the model spectral type calculations are possible. See text.

Although the ultraviolet is important for deep-atmosphere temperature profiles, no ultraviolet fluxes are output because the near-surface opacities are likely unreliable.

Table 10. Summary of key observational data on o Cet. Units: Vega magnitudes for light-curves, mJy for radio photometry, milli-arcsec for diameters.

| Wavelength (µm) | Data Type | Observation Range | Model range | Phase Coverage? | References |
|-----------------|-----------|-------------------|-------------|----------------|-----------|
| 0.55            | Light Curve | 2.5–9.5          | 2.0–11      | Y              | AAVSO, AFOEV |
| 1.2             | Light Curve | (-1.7)–(-0.3)    | (-1.8)–(-0.6) | Y              | Whitelock et al. (2000) |
| 1.65            | Light Curve | (-2.6)–(-1.3)    | (-2.6)–(-1.5) | Y              | Whitelock et al. (2000) |
| 2.2             | Light Curve | (-3.0)–(-1.8)    | (-3.0)–(-2.0)c | Y              | Whitelock et al. (2000) |
| 0.4–0.6         | Spectral Type | M5e-M9e          | Noneb        | Y              | Skiff (2009), Samus et al. (2004) |
| 0.307           | Photometry  | 14.85             | Nonec        | N              | Karovska et al. (1997) |
| 0.346           | Diameter    | 35 (FWHM)         | Noneb        | N              | Karovska et al. (1997) |
| 0.45–1.03       | Diameter    | 31–103            | 25–60d       | N              | Labeyrie et al. (1977) |
| 0.68–0.92       | Diameter    | 20–60 FWHM        | 16–38        | N              | Ireland et al. (2004) |
| 1.24            | Diameter    | 22–30             | 17–34        | Y              | Woodruff et al. (2008) |
| 2.26            | Diameter    | 31–37             | 17–29        | Y              | Woodruff et al. (2008) |
| 1.24            | Diameter    | 22–30             | 17–32        | Y              | Woodruff et al. (2008) |
| 1.1–3.8         | Diameter    | 25–68             | 17–58        | N              | Woodruff et al. (2009) |
| 11.15           | Diameter    | 46–55             | 21–72        | Y              | Weiner et al. (2003) |
| 3.6 cm³        | Photometry  | 0.20–0.37 mJy     | 0.09–0.32 mJy | N              | Reid & Menten (1977), Matthews & Karovska (2006) |
| 7 mm           | Diameter    | 52                | 29–55        | N              | Reid & Menten (2007) |

aShorter-wavelength radio observations are consistent with a ν² power law within errors. A 0.12 mJy contribution from Mira B has been subtracted.

bNo model spectral type calculations are possible. See text.
cDistance to model fixed to 107 pc so that K-band maximum agrees.
dWhen the fluorescence scattering approximation is used (as in Paper I), the range becomes 26–80 mas, with the upper diameter limited by the model 5 Rp surface.
eAlthough the ultraviolet is important for deep-atmosphere temperature profiles, no ultraviolet fluxes are output because the near-surface opacities are likely unreliable.

Let us consider how models of o Cet could be modified in order to achieve a larger apparent radius. The simplest method is to place the star at a closer distance with a lower luminosity and the same linear radius and mass (preserving the period). We note that the most recent HIPPARCOS analysis of van Leeuwen (2007) places o Cet as close as 75 pc within 2σ, which would mean luminosities as low as 2650 L⊙ are consistent with direct observations. Such a low luminosity would, however, be 0.8 magnitudes below the LMC P-L relationship (Whitelock et al. 2008). This relationship provides a stronger constraint on the absolute K-magnitude of o Cet, as the dispersion in the relationship is only 0.13 magnitudes (Feast et al. 1989). Adopting this relationship places a 2σ lower limit on the o Cet luminosity of 4400 L⊙. By solving the approximate equations 4 through 6 after decreasing the M to 1 M⊙ and increasing angular diameter by 10%, the model luminosity becomes 4200 L⊙ and the mixing length parameter αm = 2.9 (effects of αν and Z are neglected here). It is therefore likely not possible to fit all observations of o Cet unless the model mass is greater than 1 M⊙.

R Cha is a Mira variable much like o Cet (period, amplitude, colour), except for its more uncertain distance. In Section 3,
or the luminosity more than $2\sigma$ below the LMC P-L relationship – each of which would be a controversial claim. This discussion shows just how difficult it is to provide precisely calibrated models of Mira variables without clear observational reference points.

The key problem here of finding the best value for $\alpha_m$ as a function of $M$ and $L$ can be expressed as a problem of finding the radii of real stars at given $M$ and $L$. Mixing length only provides a way to calculate $R$ for given $M$ and $L$ once free parameters (especially the mixing length) are fixed based on known stars. Models of main-sequence stars and even K-giants can be calibrated very well from the sun and other stars of accurately known parallaxes. However, extrapolating to M giants, where pressure scale-heights can be a significant fraction of a radius, is not expected to be reliable.

What is therefore needed is a sample of M giants of well-known $M$, $L$ and $R$, from which to calibrate the mixing length. Although we cannot measure $M$, period can serve as a proxy for $M$ given $L$ and $R$. $L$ and $R$ can be measured accurately for a sample of stars with relatively compact atmospheres (i.e. with a well-defined $R$) that have a well-known parallax, photometry and effective temperature. At this point, spectral synthesis is not reliable enough or calibrated well enough for M giants to produce accurate effective temperatures and compositions. Therefore, this sample should include semi-regular pulsators with accurate photometry, angular diameters and periods. Either accurate periods or angular diameters are currently missing for many of the closest M giants, so we suggest that measuring and collating such information should be an active area of research.

Assuming that a reasonable value for $\alpha_m$ can be prescribed for Mira models, the main free parameters for any individual Mira are composition and $\alpha_v$. Composition (primordial metallicity and C/O ratio) must come from spectral synthesis. Given a set of Miras with well-measured distances, $L$ is determined from observations and $M$ from the period of the Mira – only $\alpha_v$ can be used to tune the model amplitude and should be relatively easy to calibrate.

6 THE MOLECULAR-SHELL SCENARIO

Interferometric measurements of Mira variables have been shown to be internally consistent only if there is a layer of molecular water far above the continuum-forming photosphere (e.g. Weiner 2004). Observational comparison with models that include this kind of water and/or dust layer have so far been dominated by non-physical models, i.e. those that neither provide a mechanism for elevating the emitting material nor calculations of the chemistry that determines which components dominate the radiative transfer at which radii.

Nevertheless, these ad-hoc models have provided a relatively simple picture for the regions around Mira variables and have impressively fitted a limited selection of observable properties. In this section we will examine the physical and observable properties of the molecular shells in our model series.

Figs. 1 to 4 show that cycle-to-cycle variations in the pulsation models are generally quite modest in terms of the luminosity, of the temperature at and the position of the $\tau_g = 2/3$ layer and of the posi-

![Figure 14. Temperature (K; upper left), density (g cm$^{-3}$; lower left panel) and the molecular density $\rho_{\rm mol}$ for molecules H$_2$O (upper right) and TiO (lower right) as a function of $r/R_p$ for 3 phases of a cycle of the o54 model series: 285180 (phase -0.20, solid line), 285860 (+0.20, dashed), 286100 (+0.49, short-dashed).](image-url)
tion of deep-layer mass zones below the $\tau_g = 2/3$ layer. The o54 and C81 model series show somewhat more pronounced cycle-to-cycle effects than the r52 and C50 models. Inspection of specific numerical values of the radius $R$ of the $T_{\text{Ross}} = 1$ layer and the therefrom derived effective temperature $T_{\text{eff}} \propto (L/R^2)^{1/4}$ given in Tabs. 2 to 8 for the non-grey atmospheric stratifications confirm this cycle stability.

In contrast, we notice substantial differences between different cycles, and often between successive cycles, in terms of the positions of high-layer mass zones (Figs. 1 to 4). These differences are closely related to substantial differences of the strengths and positions of outward traveling shock fronts. Inspection of shock-front positions (Tabs. 2 to 8) in the selected cycles for which detailed atmospheric models were computed show a shock front typically emerging at pre-maximum phase around -0.3 to -0.1, then traveling outward during about 1 to 1 1/2 cycles while it becomes weaker and slower before the subsequent front catches up and both fronts merge. Typically, the outer front starts retreating before merger, but occasional shock fronts traveling towards circumstellar space (where they eventually fade away) are also seen in the Tables.

The positions and heights of shock fronts at different phases and in different cycles determine the upper atmospheric density and, therefore, does not depend so strongly on upper-atmosphere to-cycle differences seen in the water-contaminated spectrum of the stars.

The study of Tej et al. (2003), based on models of Hofmann et al. (1998), shows that the details of shock-front propagation may lead to strong cycle-to-cycle differences of the stratification of the outer atmosphere resulting in strong differences of the density and geometric characteristics of water “shells”, i.e. of layers whose absorption is dominated by water molecules.

Figures 14 to 16 demonstrate, for the o54 and r50 series of the here presented CODEX model sets, the drastic phase and cycle effects of shock-front propagation on the temperature-density stratification and on the appearance of $\text{H}_2\text{O}$ and TiO “shells”. Density decreases monotonically with radius, while the sharp decrease at a shock front provides the outer edge of any “shell”. The decrease of temperature with radius provides a relatively sharp edge to the region where water can exist in chemical equilibrium, and this provides the inner edge of any “shell”. At most infrared wavelengths, gas is reasonably transparent between temperatures where $\text{H}$- opacity is dominant ($\gtrsim 3000 \text{ K}$) and where water is dominant ($\lesssim 1800 \text{ K}$). A similar pattern is found for the TiO molecule which, however, is formed in somewhat deeper layers than water and, therefore, does not depend so strongly on upper-atmosphere shock-fronts and shows smaller, though by no means negligible, cycle-to-cycle effects.

The model-predicted effects of such molecular “shells” upon the absorption properties of the stellar atmosphere at observationally important wavelengths have been discussed and compared to observations by Ireland et al. (2008), Woodruff et al. (2009) and Wittkowski et al. (in preparation). Figure 17 shows typical cycle-to-cycle differences seen in the water-contaminated spectrum of the
3 models presented in Figure 15. Typical effects of water “shells” upon the shape of the centre-to-limb variation have been discussed in the model study of Tej et al. (2003).

Though semi-empirical “shell” scenarios have been used with remarkable success for interpreting spectroscopic and interferometric observations of absorption features of H$_2$O (e.g. Matsuura et al. 2002; Mennesson et al. 2002; Ohnaka 2004; Perrin et al. 2004; Weiner 2004) and of TiO (e.g. Reid & Goldston 2002), models show that such scenarios can at best provide a very rough picture of the approximate instantaneous position and extent of absorbing layers. Such semi-empirical models cannot provide any information on changes of these layers with phase (since local molecule abundance and resulting molecule absorption as a function of local values of $\rho(r)$ and $T(r)$ sensitively depends on details of shockfront progression). Note also that absorption by CO in low excitation lines extends from the continuum-forming photosphere at $\sim$3000 K right to the wind region, so a CO “shell” scenario (e.g. Mennesson et al. 2002) should be considered with particular caution.

Finally, we note that the existence of shell-like structures noticeably change the computed spectra in the models, but the effects are not so strong that the detailed shell structure can be directly inferred from low spectral resolution observations. Modeling high spectral resolution observations is beyond the scope of this paper, but such a study would have to take into account the velocity structure of the atmosphere explicitly (e.g. Nowotny et al. 2010).

Figure 16. The same as Figure 14 for the same phase 0.0 of 3 models of successive cycles of the r50 model series: 375780 (-1.00, solid line), 377110 (0.00, dashed), 3783200 (+1.00, short-dashed).

Figure 17. Spectra of the 3 same-phase models of Figure 15 showing cycle-to-cycle differences of the spectrum in the J-band region of the spectrum.

7 RADIATIVE ACCELERATION AND MASS LOSS

As described in H"ofner (2008), the conditions for radiative acceleration to drive mass loss are that dust must be able to form, and that the opacity exceeds the critical opacity:

$$\kappa > \frac{4\pi c G M_*}{L_*} = 12830 \text{ cm}^2\text{g}^{-1} \left( \frac{M_*}{M_{\odot}} \right) \left( \frac{L_*}{L_{\odot}} \right)^{-1}.$$ 

(7)
This opacity is attainable at solar metallicity with fully-condensed iron-rich dust, which is not stable until approximately 5 continuum stellar radii \( R_* \). This opacity is also reached by forsterite (i.e., Fe-poor silicate) grains of 400 nm radius due to strong scattering \( \rho \) of H" ofner \( 2008 \).

The CODEX models have a chemical equilibrium model of dust formation, so are not appropriate for modeling the slowly-growing Fe-rich dust at \( \lesssim 5 \, R_* \), and indeed we artificially cut-off Si condensation at a condensation fraction of 0.25 for this reason. However, as discussed in Ireland & Scholz \( 2006 \), the prescription we use for dust formation is reasonably accurate for Fe-poor silicates.

The strongest observational constraints on the radii of dominant dust species are observations that probe the opacity at short wavelengths where dust scattering is dominant, and wavelengths where water absorption is dominant. As optically thin scattering does not affect the spectrum, the best observations to probe this difference are resolved observations of Miras as a function of wavelength. Figure 18 shows the interferometric diameters of \( \omega \) Cet as a function of wavelength as measured by Woodruff et al. \( 2008 \) along with the diameters predicted by the 286060 model and the diameters predicted by the same model with the base-10 logarithm of the number of dust nuclei per H atom \( N_{\text{nuc}} \) decreased from -12.2 to -13.7, and the corresponding maximum grain radius increased from 63 to 194 nm. These large grains still have insufficient opacity to overcome gravity in this model. We could not increase the grain radii further without the optical depths becoming too large at our chosen 5 \( R_* \) surface, and the preferred value from H" ofner \( 2008 \) of \( \log(N_{\text{nuc}})=15 \) would produce diameters that are far too large. It is clear that these large grain radii are not consistent with the relatively large \( H_2O \) column densities at several continuum radii inferred from infrared interferometric observations. Either radiation pressure on small Fe-rich grains or large Fe-poor grains could drive winds from M-type Mira variables, but the base of the wind and the grains that drive it must originate from layers higher than where \( H_2O \) is seen in the near-infrared, i.e. higher than about 3–4 continuum-forming radii.

8 CONCLUSIONS AND FUTURE WORK

The atmospheric models presented here, based on self-excited pulsation models and opacity-sampling treatment of radiation transport, provide a fairly realistic approximation of the atmospheric density-temperature stratification. Many spectral features are predicted with satisfactory accuracy but some, like TiO bands, require further improvement of the models e.g. the non-LTE treatment of Paper I. The present sequence of models also comprises only 4 combinations of basic stellar parameters at only a single composition and, therefore, can only describe a relatively small subset of Mira variables. Predictions of the 4 model series presented here (Table 1) are available on-line (Section 2.5).

There are several potential causes of substantial deviation from spherical asymmetry in Mira variables - including convective cells, weak chaos and Rayleigh-Taylor instabilities \( \text{Woodruff} \ 2008 \). Asymmetries are clearly not considered in our model series as they are spherically symmetric, but asymmetries are relatively common in Mira variables when observed at sufficient angular resolution (e.g. \( \text{Ragland} \ et al. \ 2006 \)). The one prediction that can be made from the models is that the wavelengths most susceptible to cycle-to-cycle variations (e.g. I-band where the water shells are optically-thick) should also show asymmetries, as high layers on opposite sides of the star should not be strongly causally connected and show weak chaos. We finally suggest that an observation so far missing in the literature is the astrometric motions of the radio photosphere over several cycles, which should be a strong indicator for the degree of high-layer chaos in Mira atmospheres.

Determination of the internal fundamental model parameters, i.e. mixing-length \( \alpha_{\text{m}} \) and turbulent viscosity \( \alpha_{\nu} \) (Table 1), would require observation of a set of stars with different mass, luminosity and pulsation period. For a given pulsation period, a higher-mass star must have a higher luminosity (radius), but a similar effective temperature. We suggest that further studies of low-amplitude pulsators with Mira-like periods such as R Dor and W Hya may provide the key to tuning the mixing length parameter \( \alpha_{\text{m}} \) of Mira model series. These are likely higher-mass stars, but with a similar effective temperatures to \( \omega \) Cet. Tuning the turbulent viscosity parameter will best be done by fitting to amplitudes of models with the best-known masses such as, e.g., those kinematically associated with the thick disk.

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Figure 18. Interferometric diameters for the \( \omega \)4 series model 286060 (phase 0.41), fit to the spatial frequency where visibility \( V = 0.5 \). The solid line corresponds to the default number of dust nuclei, and the solid red line corresponds to a factor of 3.1 increase in grain radius, at log(N_{\text{nuc}})=13.7. Observations from Woodruff et al. \( 2008 \) at phase 0.3 are over-plotted. Despite still not being able to drive a wind, the large diameters at short wavelengths are clearly inconsistent with observations.
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