MODELLING NIR MOLECULAR LINES FOR MIRAS

Walter Nowotny¹, Susanne Höfner², Thomas Lebzelter¹, Bernhard Aringer¹, Josef Hron¹

(1) Institut für Astronomie, Universität Wien, Austria
(2) Dept. of Astronomy and Space Physics, Uppsala University, Sweden

email: nowotny@astro.univie.ac.at
BASIC FACTS ABOUT MIRAS

A) pulsating red giants on the Asymptotic Giant Branch (Miras) have extremely extended atmospheres (≈AU, several 100 R_☉), which are heavily affected (e.g. gas velocities) by pulsation, dust formation and mass loss

B) lines of various molecular lines/bands have different excitation energies/temperatures → originate from different depths, show diverse behaviours

C) time series of high-resolution NIR-spectroscopy:
   – study (molecular) line profiles
   – derive radial velocities (RV) from Doppler-shifted lines

A+B+C ⇒ study dynamics throughout outer layers of AGB stars

CO especially useful for this purpose: e.g. observations of χ Cyg by Hinkle, Hall & Ridgway (1982) abundant in all types of chemistries (M/S/C), stable over whole atmosphere + large parts of CSE, no depletion into dust, 3 types of vib-rot bands with different exc. energies observable (atmospheric windows)

for C-rich Miras also CN – observations of S Cep by Hinkle & Barnbaum (1996)

⇒ reproducing the time-dependent behaviour is a major challenge for dynamic models:

i. for interpretation of complex multi-component line profiles (caused by non-monotonic velocity fields) → better understanding of atmospheric kinematics

ii. fundamental test for quality of models
aim: reproducing the complicated atmospheric structures + variations properly, in particular dynamic phenomena such as Doppler-shifted spectral features

- consistent models from photosphere out to dust forming region and beyond to stellar wind regions (Höfner et al. 2003)

- simultaneously solved: – hydrodynamics
  – frequency-dependent radiative transfer (51 points in λ, molecules)
  – time-dependent treatment of formation and evolution of C-rich dust (amorphous carbon only)

- pulsation of interior simulated by variable inner boundary below photosphere (piston with velocity amplitude Δu_{piston})

parameters of the models used: (hydrostatic initial model – piston parameters – resulting mass loss)

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<td>Modell A</td>
<td>10^4</td>
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<td>493</td>
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<td>Modell B</td>
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<td>1.4</td>
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<td>2.5 \cdot 10^{-6}</td>
<td>7.5</td>
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models represent observed low-resolution spectra of AGB stars from visual/red to MIR rather well, as shown by Gautschy-Loidl et al. (2004)

phase shift between bolometric phases φ_{bol} (used to denote computations) and visual ones φ_{V} (as used in observations) for models not investigated yet
characteristics of the models: Figs. 1+2
spherical symmetry assumed (1D)
complicated atmospheric structures, strongly differing from hydrostatic models (initial model, MARCS)
  - shallow global density gradient, very extended atmosphere
  - strong local variations ($\rho$, $u_{gas}$), spatially/temporally (shock fronts, dust shells)
  - mass loss (dust-driven wind)
C-rich chemistry:
  dust-formation process better understood than for O-rich case $\rightarrow$ consistent modelling possible

SPECTRAL SYNTHESIS

complex line formation:
  contributions from layers with various conditions $-$ especially velocities (incl. projection effects)
synthesis of selected molecular lines, which probe different regions within atmosphere $+$ wind

• equilibrium chemistry for chemical abundances $+$ LTE assumed
• special opacity treatment: (cf. Nowotny et al. 2005a)
  – molecular opacities from line lists of CO, CN
  – other molecular species (esp. C$_2$H$_2$) approximated by OS
  – dust opacities included (pure amorphous carbon, no SiC)
• detailed radiative transfer: in spherical geometry, including velocity effects (essential)
• computed with resolutions of $\lambda/\Delta\lambda=300.000$, rebinned to 70.000 (comparable to observed FTS spectra)

$\Rightarrow$ RVs derived from wavelength shifts of the synthetic lines
results published in Nowotny et al. (2005a, 2005b, 2005c)

model parameters:
  chosen to resemble S Cep (typical carbon-rich Mira, only one with time series spectroscopy)
  but not a specific fit

- **CO $\Delta v=3$ and CN $\Delta v=-2$ (red system) lines:**
  originate in deep photosphere dominated by pulsation ($\approx 2200-3500$ K)
  computed: CO 5–2 P30 at 1.65$\mu$m (H-band) and CN 1–3 Q$_2$ 4.5 at 2.05$\mu$m (K-band)
  layers modulated periodically $\rightarrow$ line profiles repeat every pulsation period
  model spectra reproduce observed variation of line shape for the lower spectral resolution (70.000)
  (profiles appear more complex at highest resolution – but no observations possible so far)
  line doubling at certain phases $\rightarrow$ evidence for shock front propagating through line-forming region
  typical discontinuous, S-shaped RV-curve also reproduced
  CN lines originate a little further out – suggested by small shift of RV curve

- **CO $\Delta v=2$ (low-excitation) lines:**
  originate in dust forming region, where stellar wind is triggered ($\approx 800-1500$K)
  computed: 2–0 R19 at 2.31$\mu$m (K-band)
  velocities not periodic – agreeing with obs. (different timescales of pulsation and dust formation interfere)
  multi-component profiles: variability less pronounced than for CO $\Delta v=3$, no clear line doubling,
    but several components (not separable, variable in number and intensity) $\rightarrow$ broad asymmetric shapes;
    some variation over lightcycle, not coupled with pulsation
  RV always slightly blue-shifted (low outflow) $\neq$ observations (small variations around CMRV, i.e. RV=RV$_*$)
• **CO \( \Delta v=1 \) lines:**
  
  originate in wind region \((\approx 350-500 \text{K})\)
  
  computed: 1–0 R1 at 4.65\( \mu \text{m} \) (M-band)

  stationary outflow, only small changes of terminal velocity on timescales longer than pulsation period
  
  P Cyg–type profile at any instance of time (characteristic for lines formed in wind)
  
  deep blue-shifted absorption with wind velocity (outflowing layers in front of star)
  
  slightly red-shifted emission (extended region around the star)
  
  observationally difficult spectral region (telluric absorption)

**summary:**

... dynamic models ...

... seem to have atmospheric structures \((T_{\text{gas}}, \rho_{\text{gas}}, \text{etc.})\) very similar to real Miras

... have on top of that a global velocity structure in qualitative agreement

... allow qualitatively to reproduce the scenario by consistent calculations:
  
  – probing dynamics in layers of different depths by various molecular lines
  
  – simultaneously by one model
  
  – profiles (line shapes, depths, doubling, etc.) reproduced
  
  \( \Rightarrow \) behaviour of RVs resemble observational results for Miras

\( \Rightarrow \) models show fundamental agreement with dynamic processes occurring in Miras

**but:** qualitatively some differences remain

\( \text{e.g. amplitude of RV curves of CO } \Delta v=3 / \text{CN } \Delta v= -2\) lines \( \Rightarrow \) Model B ...
Fig. 3: Complex line formation - Model A

![Graph](image)

- **$v_{gas}$**
- **$\rho_{gas}$**
- Pulsation
- Dust formation
- Dust shell
- Onset of wind
- Outflow
- Infall
- Shockfront

Radius $R$ ($R_*=493R_\odot$) vs. velocity $u_{gas}$

Sub-plots:
- CO $\Delta\nu=3$
- CO $\Delta\nu=2$
- CO $\Delta\nu=1$

RV [km/s] vs. $F/F_{cont}$
Fig. 4: Radial velocities derived from synthetic line profiles of different molecular lines – Model B

![Graph showing radial velocities vs. phase for different molecular lines.](Model_B_plot)

- **Infall** = red-shift
- **Outflow** = blue-shift
RESULTS FOR MODEL B – TOWARDS REALISTIC MODELS

Fig. 6 – left panel:
- compilation of CO $\Delta v=3$ RV measurements for all Miras observed so far (data taken from Hinkle & Lebzelter 2002)
- very typical S-shaped RV-curve (grey thick line to guide the eye)
- amplitude of $\Delta RV = 20-30$ km/s
- rather uniform picture for all stars independent of spectral type, period or metallicity

fundamental characteristic of Miras $\rightarrow$ realistic models have to reproduce this!

Model A: Nowotny et al. (2005a)
- ☑ observed behaviour of CO $\Delta v=3$ lines qualitatively reproduced
- ☹ velocity jump in shock front too low
  $\rightarrow$ line splitting too weak + extracted velocity amplitude $\Delta RV$ too low $\rightarrow$ compared with observations

new Model B:
- parameters tuned to fit this aspect
- higher piston velocity $\rightarrow$ variability of atmospheric structure more pronounced in the inner parts
- more compact ($\lg g, \uparrow$) $\rightarrow$ lower outflow velocity and mass loss rate

Fig. 5: left: observations of $\chi$ Cyg from Lebzelter et al. (2001)
- averaged line profiles from 10-20 lines in FTS spectra, plotted vs. observed visual phase $\phi_v$
- $\chi$ Cyg taken as representative Mira (lack of data for S Cep or any other C-rich Mira)
- RVs relative to CMRV

right: synthetic line profiles for CO 5-2 P30 line, plotted vs. bolometric phase $\phi_{bol}$ of model
top spectrum computed without taking velocities into account
conclusions: Fig. 6 – right panel

CO $\Delta v=3$ RV-curve for first time also quantitatively reproduced!

S-shape, line-doubling interval, zero-crossing phase, asymmetry w.r.t. RV=0: infall velocities $>$ outflow velocities – as observed in most Miras
and (mainly) $\Delta RV \approx 21$ km/s: more extreme velocity gradient across the shockfront
$\rightarrow$ line-doubling more pronounced than for Model A

synthetic RV-curve shifted in phase to fit $\rightarrow$ suggests a phase shift of 0.3 between $\phi_{bol}$ and visual phases $\phi_v$ for the model, such that $\phi_{bol}$ lags behind

$\Rightarrow$ dynamic model atmospheres approach quantitative agreement with observations

References:

"Atmospheric dynamics in carbon-rich Miras I. Model atmospheres and synthetic line profiles"
"Atmospheric dynamics in carbon-rich Miras II. Models meet observations"
Nowotny, Aringer, Höfner et al. 2005c, ESO Astrophysics Symposia, Springer, p.283
"Synthetic line profiles for pulsating red giants"
Fig. 5: Comparison of observed line profiles with synthetic ones of Model B
Observed radial velocities – all Miras, CO $\Delta v=3$

Synthetic radial velocities – CO $\Delta v=3$

Model A
Model B

Figure 6
Poster „Modelling NIR molecular lines for Miras“
Nowotny et al. 2005
Pulsationstagung in Rom/Monte Porzio, Juni 2005

Anordnung der Seiten: ausgelegt auf Platz von 1.5m*1.2m (H*B)