Project B1: The radiation-hydrodynamics of photoevaporative winds with chemistry

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Requested positions: 1 Postdoc

Abstract:

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Type 1 TDs are most likely discs in an advanced stage of dispersal (see introduction to the Research Unit). The dispersal mechanism of discs has been shown to be of fundamental importance to planet formation, yet the responsible mechanism is still largely unconstrained. Photoevaporation from the central star is currently a promising avenue to investigate, but the models developed to date do not yet have enough predictive power for a piecewise comparison with the observations. We aim at building the most up-to-date radiation-hydrodynamical calculations of irradiated discs, coupled to photoionisation, chemistry and radiative transfer calculations. This will constitute the backbone for the work carried out in several sub-projects of this proposal (B2, C2), which together aim at performing quantitative spectroscopy of disc winds. Comparison with existing and upcoming observations will allow us to constrain the mass loss rates and the launching regions of the wind and thus pin down the underlying driving disc dispersal mechanism.

1. State of the art and preliminary work

1.1 Scientific Background

Understanding disc dispersal is a key piece in the puzzle of planet formation. Type 1 TDs, which are considered to be objects caught in the act of dispersal provide a tight constraints on the underlaying dispersal mechanism. For example, their (low) frequency, in relation to the global disc population in a given cluster, implies dispersal timescales of order 10% of the global disc timescale, and their evolution on the colour-colour plane points to an inside-out mode of dispersal (e.g. Ercolano, Clarke & Hall, 2011; Koepferl, Ercolano et al. 2013; Ercolano et al. 2015).

The most successful of the various disc dispersal mechanisms proposed to match many of the observational constraints is photoevaporation by radiation from the central star (e.g. Clarke et al. 2001). As described in more details below, once the mass loss rate due to photoevaporation exceed the mass accretion rate through disc, the wind can quickly destroy the disc, eroding from the inside-out.

Recent work suggests that magnetohydrodynamic (MHD) turbulence may also drive disc winds (e.g. Bai & Stone, 2013), which may lead to disc dispersal and at the same time remove angular momentum from the system, thus allowing the inward flow of material, i.e. accretion. These models are still in their infancy and the mass loss and accretion rates from MHD winds are at present highly uncertain. What is certain, however, is that if MHD winds are indeed as vigorous as some authors claim, they would completely change the way we understand disc evolution and dispersal, invalidating may of the models that are based on alpha-type discs. Some of the main sources of uncertainty include the strong dependence of the wind and accretion rates on the completely unknown magnetic flux distribution through the disc and, most importantly, magnetic flux evolution as a function of surface density of the disc (e.g. discussion in Armitage et al. 2013). Another key ingredient is the level of ionisation in the atmosphere of discs, which determine the nature of the gas coupling to this unknown magnetic field. While details of the magnetic field structure and evolution are difficult to determine at present, the joint efforts of sub-projects B1, B2 and C2 can deliver the most detailed assessment to date of the ionisation structure in disc atmospheres. This is indeed one of the aims, which is described in subproject B2 (PI: Caselli).

In the following two sections the state-of-the art for photoevaporation models and for current disc wind tracers will be discussed.

1.1.1 Photoevaporation models

All models of photoevaporation show that radiation from the central star heats the disc atmosphere, where a thermal wind is established. The wind is centrifugally launched from the location where the thermal energy of the heated gas exceeds the local gravitational binding energy. Disc dispersal then sets in as a consequence of the wind when the mass loss rate exceeds the accretion rates in the disc. According to viscous theory, young discs accrete at a vigorous rate, which naturally decreases as time goes by (REF?????), until, after a few million years accretion rates fall to values smaller than the wind rates, allowing photoevaporation to take over the further evolution of the disc. Once the dispersal sets in the disc is then quickly eroded from the inside out (see e.g. Alexander et al. 2014 and Armitage et al. 2011, for recent reviews of this process).

While the community now agrees on this broad brush picture, quantitatively speaking, the dispersal mechanism is still largely unconstrained. There is currently a hot debate in the literature as to what type of radiation may be the main driver of the wind: Extreme-, Far-UV or X-ray. This is a fundamental question as the mass-loss-rates implied by the different models can differ by orders of magnitudes. Mass loss rates determine the timescales of dispersal for given initial disc conditions. The wind profile, i.e. the region of the disc that is most affected by photoevaporation, is also very different in each scenario (e.g. see Armitage 2012, Alexander et al. 2014). Figure ??? shows the mass loss profile for the X-ray+EUV (Owen, Ercolano et al. 2010), EUV -only (Font et al. 2004) and FUV (Gorti, Dullemond & Hollenbach 2009) profiles. The X-ray profile is more extended than the EUV profile, which predicts mass loss only from a vary narrow range of disc radii. The FUV model is again very different, showing mass loss from the outer regions of the disc, hence predicting in some cases an outside-in mode of dispersal. The total mass loss rates in the disc sets the timescales for the formation of gas giants, while the wind profiles sculpt the disc density distributions, profoundly affecting the evolution of all planetary systems, by putting a stop to migration via the formation of gaps in the gas. As an example, we have shown that the photoevaporation profile strongly influences the final semi-major axis distribution of exo-planets (Ercolano & Rosotti, 2015)

All models are incomplete. Some models focus on hydrodynamics and assume isothermal gas (e.g. the EUV-olny model of Font et al. 2004), others focus on chemistry but do not perform hydrodynamical calculations (e.g. the FUV model of Gorti, Dullemond & Hollenbach 2009). None of the existing models take into account dust evolution in the underlying disc and entrainment of grains in the wind. Together with my previous PhD student, I performed the only existing radiation hydrodynamic calculations of X-ray + EUV driven winds to date (Owen, Ercolano et al. 2010, 2011a, 2012), using realistic gas temperatures obtained from X-ray photoionisation calculations (Ercolano et al. 2008, 2009). This led to a fundamental re-think to the whole problem, as previous isothermal calculations had yielded much lower mass loss rates (by two orders of magnitude). However, our models, which still represents the state-of-the-art, also have crippling limitations, since, most importantly, they do not include chemistry and ignore the dust phase. Furthermore the resolution at which the simulations were performed is insufficient to study lines with emission regions extending close to the disc inner edge. These limitations make the application of current models to observations impossible.

1.1.2 Disc Wind diagnostics

The fundamental reason why the theoretical models still wildly disagree with each other is because until now they could not be directly tested with observations.

The presence of disc winds has been confirmed via the observation of a few km/sec blue-shift in the line profiles of a number of tracers like [NeII] 12.8μm and [OI] 6300 (e.g. Pascucci et al 2007, Rigliaco et al. 2013) and a number of collisionally excited lines in the optical region (Natta et al. 2014). Figure 1, taken from an upcoming review on transition discs by Ercolano & Pascucci (2017, to appear in Royal Society Open Science) shows an example of possible wind diagnostics.

We have demonstrated, however, that the [NeII] 12.8μm and the optical forbidden lines cannot be used to infer the underlying mass-loss-rates (e.g. Ercolano & Owen 2010, Ercolano & Owen 2016). For example, the intensity and the profile of the [NeII] 12.8μm line can be equally well fitted using an EUV (Alexander 2008) or an X-ray photoevaporation model (Ercolano & Owen 2010), as shown in Figure??????. The problem with the [NeII] line is that the Ne+ formation route can occur both via the removal of a valence electron in the fully-ionised winds driven by EUV radiation, but also by charge exchange of Ne++ with neutral H which is abundant in the quasi-neutral winds driven by X-ray. The problem with the [OI] 6300 line and all other optical collisionally excited lines considered to date is the strong temperature dependence imposed by the Boltzmann term in the emissivity. This means that these lines are mostly just tracing the hot layer of the wind heated by the EUV radiation and not actually tracing the bulk of the wind where it matters (Ercolano & Owen 2016), hence they cannot be used to infer mass-loss-rates or to constrain the wind driving mechanism.

This picture was further complicated by the recent high spectral resolution observations of Simon et al. (2016) who found that low velocity emission in [OI] forbidden lines, classically attributed to a slow-moving disc wind, is present in all T-Tauri stars with dust disks, even those classified as WTTs, but it is best fit by a superposition of a broad and a narrow component. Most of the broad component emission arises within 0.5AU and Simon et al. (2016) interpret it as being produced in a magnetically driven wind, given that the emitting region is well inside the gravitational potential well of the central star. The narrow component, which, unlike the broad component, is always present in also in transition discs, traces gas further away (0.5-5 AU) and is probably associated with photoevaporative winds.

The interpretation of the broad component as a tracer of a magnetic wind is however problematic for a number of reasons. The main problem is that one would need a very large scale height to overcome the fact that the emitting volume dominates as one goes to larger radius. Presumably a very large magnetic pressure would be needed to achieve this. Furthermore, if an hypothetical magnetic wind would have enough density to match the observed broad component, it may also absorb out all UV flux, which would then not be available to irradiate the wind at larger radii, which is clearly indicated in the observations.

An alternative explanation could be that the broad component is not produced in the wind, but is emitted by bound material in the disc itself. The broad component, if coming from the inner disc, cannot have however a thermal origin. We have tested that with a new higher resolution set of hydrodynamical calculations, similar to those presented by Ercolano & Owen (2016), which extend further into the inner disc, to $r_{\rm in}$=0.04 AU. The line profiles for the high resolution hydrodynamical calculations are shown in Figure ???? for R=25000, which represent the resolution of the Rigliaco et al (2013) data, when the two component had not been resolved yet, and R=50000, which is more representative of the work of Simon et al. (2016). The R=50000 line profiles in our simulations do show broad wings at high disc inclinations. The wings are due to bound material in the inner disc. However the wings from our high resolution models are still much smaller (i.e. do not carry enough flux) than those detected by Simon et al. (2016). In fact in our calculations the line flux is completely dominated by the (unbound) emission at larger radii. This is easy to understand as the flux is proportional to density squared times the volume and the volume for an isothermal region in the disc scales like $R^{7/2}$ ($R^2 \times H$). Given that the density does not fall off steeply enough in the heated region then the emission at larger radii dominates. For example a density profile set by the absorption of photons to a fixed column - indicative of our case - would fall of approximately as $n \propto 1/R$, provided the absorption is dominated at large radius.

Our calculation show nevertheless that bound material in the very inner disc can indeed produce broad wings. If the column of emitting bound material were larger then stronger wings would be produced. A non-thermal process acting at higher columns in the inner disc, as for example dissociation of the OH molecule (Gorti et al. 2011), could indeed produce the missing flux in the wings. As our codes currently lack chemistry we have been unable to test a non thermal origin of the broad component. This is however an important task, as if confirmed, there would be no need to invoke magnetic disc winds to explain the observations.

Mid-infrared observations of molecular lines (e.g. CO) provide a new promising alternative to directly measure disc winds. Indeed recent observations suggest that these lines may be tracing a disc wind which is slow and partially molecular (e.g. Pontoppidan et al. 2011; Brown et al. 2013). The spectro-astrometric survey of molecular gas in the inner regions of protoplanetary discs using CRIRES, the high-resolution infrared imaging spectrometer on the Very Large Telescope (Pontoppidan et al. 2011), showed that for several sources the astrometric signatures are dominated by gas with strong non-Keplerian (radial) motions. These authors concluded that the non-Keplerian spectro-astrometric signatures are likely indicative of the presence of wide-angle disc winds. More observations of this type are planned after the update of the CRIRES instrument, which is expected to be completed by 2019. Observations with ALMA in molecular lines like e.g. CO J = 2-1 and J = 3-2 emission are also able to trace the presence of a wind (e.g.Klaassen et al. 2013, 2016). Molecular lines are sensitive to the mass loss rates since they sample a significant area of the wind launching regions. However the exploitation of molecular tracers is currently severely hampered by the lack of a suitable hydrodynamic wind model coupled to chemistry and to dust evolution models (which dominate the opacity in the wind) to interpret the observations.

While a number of chemical models exist of the deeper, denser regions of discs, no model is currently available for the optically thinner disc winds. The work of Gorti & Hollenbach (2009), while carrying out detailed chemical calculations extending to the disc atmosphere, used a hydro*static* disc model which was analysed in a 1+1D fashion. Without hydro*dynamics* no predictions on line profiles can be made.

Studying the kinematic of the emitting gas is the only way to constrain the origin and intensity of the disc wind and hence shed light on the driving mechanism behind the dispersal of discs and the formation of Type 1 transition discs.

1.2 Preliminary work

The determination gas temperatures in a photoionised gas, in a photodissociation region (PDR) or in an X-ray dissociated region (XDR) is computationally expensive. It requires, first of all performing a radiative transfer (RT) calculation in order to determine the radiation field at each point of the region. Then matrices of thermal and ionisation balance and/or rate equations have to be solved. The RT and the balance/rate equation are often coupled through the temperature-dependent gas opacities. There is a host of microphysics that needs to be taken into account, last but not least the thermal coupling of the gas and the dust phase. Even a extremely simplified version of the above results crippling if it needs to be performed at every time-step of a hydrodynamical calculation.

In such cases it is convenient to look for parameterisations of the gas temperature in terms of quantities that are easy to determine in the hydrodynamics code (e.g. gas properties and/or column density). Indeed using such a temperature paremeterisation, determined via detailed X-ray photoevaporation models using the MOCASSIN code (Ercolano et al. 2008, 2009) we have performed the only existing radiation hydrodynamic calculations of X-ray + EUV driven photoevaporative winds to date (Owen et al. 2010, 2011, 2012). The models were run with a version of the ZEUS2D code which was modified by us to include a temperature scheme derived from the detailed X-ray and EUV photoionisation calculations of protoplanetary discs of Ercolano et al. (2008, 2009). In this work it was shown that, within the penetration depth of ∼1keV X-rays ($\sim 10^{22} cm^{-2}$), the temperature of a parcel of gas with hydrogen number density, n_H, at distance r from the central star, could be roughly approximated by a function of the ionisation parameter, defined as $L_X/(r^2 n_H)$, whereL_X is the stellar X-ray luminosity. The error on the temperature is small for high ionisation parameter values, but it becomes systematically larger at the low end.

As the gas temperature enters the hydrodynamics via the square root dependance on the sound speed, the small error at high values of the ionisation parameter, typical for the regions where the bulk of the wind is driven from in primordial discs, is unlikely to produce large uncertainties in the mass loss rates. For more evolved objects, like transition discs in the phase of final dispersal, however, the ionisation parameter decreases dramatically as the cavity becomes larger. The evolution of transition discs depends thus sensitively on the temperature of the gas at low ionisation parameters, which is currently poorly represented by the parameterisation of Ercolano et al. (2008, 2009). Note that the recent work of Haworth, Clarke & Owen (2016) presents a form of the temperature ionisation parameter relation which is incorrect at low values of the ionisation parameter. The kink at ionisation parameters just above 10^{-7} (left panel of Figure???) is an artefact of their implementation of the photoionisation models. We have recently performed new detailed photoionisation calculations and obtained the curve shown in the right panel of Figure???? (Ercolano, Picogna & Owen, 2017). Our collaborators J. Owen and C. Clarke, have been informed of the problem and agree with our more recent calculations. Furthermore we have now found a more accurate scheme that allows us to reduce the error on the temperature by introducing column density as an additional parameter.

As well as the major shortcoming highlighted above, the Owen et al. (2010) calculations which were used to make predictions on the ionised phase of the wind spectra (Ercolano & Owen 2010; Ercolano & Owen 2016), suffered from low spatial resolution, precluding us from being able to model the inner region of the bound disc, which may be relevant to interpret the broad wings presented in the recent work of Simon et al. (2016). Furthermore, a very limited parameter space was investigated, which included only two values for stellar mass, 3 values of X-ray luminosity for primordial discs and a single stellar mass and X-ray luminosity value for transition discs with 3 values for the cavity radius. This is nowhere near enough to draw any significant conclusions about trends in possible wind diagnostics.

1.3 Project-related publications

1.3.1 Articles published or officially accepted by publication outlets with scientific quality assurance; book publications

[Text]

1.3.2 Other publications

None

1.3.3 Patents

1.3.3.1 Pending

None

1.3.3.2 Issued

None

2. Objectives and work programme

2.1 Anticipated total duration of the project

36 months

2.2 Objectives

The overarching aim of this project, in common with projects B2 (PI Caselli) and C2 (PI Ercolano), is to identify new wind tracers and use them to constrain mass loss rates and hence disc dispersal models, leading to the formation and evolution of Type 1 transition discs.

The new comprehensive radiation-hydrodynamics photoevaporation models developed in this project will enable a quantitative spectroscopic evaluation of new diagnostics of disc winds, via detailed astrochemical models developed together with project B2, using the dust model for the wind and atmosphere from project C2.

We will perform a comparison between TDs and primordial disc to provide important constraints on the wind architecture and the mechanism driving the dispersal. Type 1 TDs, are particularly interesting as the streamline architecture of their winds and the profiles of the lines that are produced in the wind differ from those of primordial discs. (e.g. Ercolano & Owen 2010, Ercolano & Pascucci, 2017, in preparation). Indeed the lines are expected to be broader and brighter for e.g. inner cavities of a few to 10 AUs.

The immediate objective of project B1 is to produce a new set of X-ray+UV photoevaporation models which goes well beyond the current state-of-the-art, described in the previous section.

The new models will constitute the backbone for the joint investigation to be carried out in projects B2 and C2, as well as allowing us to address the following important unsolved questions in the formation of Type 1 transition discs and their further evolution:

1. How fast do Type 1 TDs evolve/disappear after the inner disc has drained?
2. How does the formation & evolution of Type 1 TDs scale with stellar mass and stellar emission properties?
3. What is the role of FUV heating in the late evolution of Type 1 transition discs?

2.3 Work programme including proposed research methods

In this project we will significantly expand on the state-of-the-art of these widely used photoevaporation calculations by constructing a library of high resolution X-ray+EUV wind solutions for an extended grid of X-ray luminosities and stellar masses, covering all observed values. Our new calculations will make use of a new temperature scheme (Ercolano, Picogna & Owen, 2017, in preparation), derived from new more extensive X-ray + EUV photoionisation models. The new temperature scheme significantly reduces the error at low ionisation parameter values, allowing us to make solid predictions of the late evolution of transition discs.

Furthermore, our previous calculations (Owen et al. 2010, 2011, 2012) could only account for heating in the ionised phase of the wind, ignoring that the region beyond the layer heated by the soft X-ray

($< 1keV$) could be heated by FUV radiation with typical PDR or XDR characteristics. While we show in Owen et al. (2012), that this should not affect the mass loss rates at around 1-10 AU, the effect of FUV heating at larger radii may be important. We have recently coupled our 3D X-ray and EUV Monte Carlo photoionisation code MOCASSIN to the KROME package to solve the chemistry in the deeper layers of the disc (Ercolano & Grassi, 2017, in preparation). The code has been benchmarked for a simple toy network, but we will need input from project B2 to include an appropriate network to model this region and devise a new temperature scheme to include in our radiation-hydrodynamic simulations.

Note that we do not plan to run a full parameter space grid including the effects of the FUV heating. Our simulations will be limited to a selected number of cases aimed at specifically testing how strongly, and for what initial conditions, FUV heating may affect the evolution of the outer regions of discs, in particular of those in transition. Indeed one of the problems with current photoevaporation models is the prediction of a large number of non-accreting transition disc with large holes (e.g. Owen ?????REF). In this project we will be able to test the suggestion that FUV heating may take over the late-stage evolution of transition discs, speeding up their final complete erosion. Our models of the PDR in the inner disc regions will also allow us to investigate a possible non-thermal origin for the broad component of the low-velocity component of the forbidden [OI] emission, detected by Simon et al. (2013) and attributed to a magnetically driven winds.

2.4 Research Tools

For this project we will need the following tools:

1. A hydrodynamical code which we will modify to include the effects of X-ray + EUV irradiation as we did in Owen et al. (2010). For that we will use the Pluto code, for which extensive expertise exists in our team.

2. A photoionisation and chemical code which includes X-ray heating and ionisation to obtain a new comprehensive temperature scheme for the radiation-hydrodynamic simulations. The PI is the author of the 3D Monte Carlo photoionisation and dust radiative transfer code MOCASSIN (Ercolano et al. 2003, 2005, 2008b), which has already been used to calculate the emission line spectra from the ionic phase of X-ray winds (Ercolano & Owen 2010; 2016). The code has now been coupled and benchmarked to the KROME code to perform arbitrary chemical calculations (Ercolano & Grassi 2017, in prep) and needs now only the appropriate chemical network, which we will obtain from project B2.

2.5 Research Plan

We have divided the work load into two connected blocks which also have self-contained immediate objectives. Preparatory work for Block 1 is already being executed by Dr Picogna, employed on a LMUExcellent initiative grant awarded to the PI in support of this Research Unit application (End date November 2017). In case of an award Dr Picogna has already agreed to continue his work for the Research Unit and will take over the tasks described in Block 1.

A grid of significantly improved new photoevaporation models including an accurate temperature scheme which includes X-ray, EUV and FUV heating will be developed in Block 1, by means of radiation-hydrodynamic calculations. Block 2 will provide a new temperature scheme for the hydrodynamical calculations of Block 1, by performing detailed photoionisation calculations with simple chemistry using the MOCASSIN+KROME code. The PI will take full responsibility of the tasks described in Block 2 and will work closely with Dr Picogna for the implementation of the results in Block 1.

2.5.1 Block 1: New state of the art radiation-hydrodynamic models of photoionised winds.

2.5.1.1 Preparatory work: present until beginning of the award

The hydrodynamical code PLUTO (REF???) is being modified to include the effects of X-ray and EUV irradiation using the temperature-ionisation parameter from Ercolano et al. (2008,2009) also employed by Owen et al. (2010) for the ZEUS2D calculations. The obtained solutions will be first of all benchmarked against those that are already available for a 0.7 and 0.1 $M_\odot$ central stars (Owen et al. 2010, 2011, 2012), for similar spatial resolution. This will ensure that we have implemented the algorithm correctly in PLUTO.

2.5.1.2 Months 1-12

We will then proceed with the implementation of the new, more accurate temperature scheme described in the previous Section (Ercolano, Picogna & Owen, 2017, in preparation). We will compare the resulting wind rates and profiles for the primordial and transition disc case. While we do not foresee large changes in the rates for primordial discs, as described in the previous section the evolution of transition discs will be most likely affected.

The new models will have much higher spatial resolution extending much closer into the star, in order to allow tracking profile components which may be emitted from the inner bound atmosphere of the disc.

This first set of models for $\sim$solar mass stars at a typical X-ray luminosity ($\sim 10^{30}$erg/sec) will be then passed on to projects C2 and B2 for the dust and detailed chemistry calculations.

2.5.1.3 Months 13-24

The parameter space of the calculations will be then significantly extended for the mass of the central star and its X-ray luminosity. Furthermore models of transitions discs at several stages of evolution, as tracked by the radius of their inner cavity, will be performed.

With the new models we will also be able to investigate how the process scales with stellar mass and stellar emission properties. This will allow us to check the theoretical relations for X-ray photoevaporation predicted by means of semi-analytical models and ab-initio arguments by Owen et al. (2012). While these relations are being widely used in the literature, they have until now never been tested.

2.5.1.4 Months 25-36

At this point a new temperature scheme, including the effects of FUV heating, should become available from Block 2. It is likely that a streamlined form of radiative transfer will be needed in PLUTO at this point, meaning that these calculations will probably be more expensive to run. Implementation of an efficient radiative transfer algorithm in PLUTO will be carried out together with the PI (see Block 2).

However, as described above, only a limited number of calculations are planned that include this effect. These will allow us to assess the relevance of the FUV in the very final phases of disc dispersal and at large radii, where X-rays are weak.

If time allows, as a further step we plan to perform a very small set of 3D simulations to explore the effects of asymmetries in the inner disc. We expect to see dramatic effects in the photoevaporation profile and in the wind architecture, which may lead to the formation of large hole TDs. This avenue is never been explored before. It is however likely that a more comprehensive study of this effect will have to be delayed until the second funding period.

2.5.2 Block 2: Efficient temperature schemes from detailed photionisation and chemistry calculations.

The work described in this section will be performed directly by the PI, who plans to dedicate 20% of her research time to perform the tasks below within the given timescales.

2.5.2.1 Preparatory work- present until beginning of the award

As mentioned in the previous section we have significantly improved on the original parameterisation of the gas temperature, by performing new detailed calculations which are now described in terms of gas column as well as ionisation parameter (Ercolano, Picogna & Owen, 2017, in preparation). We are currently working at optimising the interpolation curves for our results, to further minimise the error on the temperature, and are confident that the new prescription will be ready by the beginning of the award.

Furthermore the PI has been working on coupling her 3D Monte Carlo photoionisation and dust radiative transfer code MOCASSIN (Ercolano et al. 2003, 2005, 2008b) to the KROME package (Grassi et al. 2014), to perform arbitrary chemical calculations (Ercolano & Grassi, 2017, in preparation). Simple photoionisation benchmarks from the set of Ferland et al. (????) have already been successfully performed with the new coupled version, and a very basic chemical network has also been introduced. This is however inadequate for any realistic modelling of disc chemistry.

2.5.2.2 Month 1-18

We will work in collaboration with the group of Prof. Caselli (B2) on introducing a reduced chemical network into our MOCASSIN-KROME code, which captures the temperature distribution obtained by the more extensive chemical modelling performed in project B2. The code will then be used to obtain a new parameterisation of the gas temperatures that can describe the physical conditions in the PDR and XDR regions.

While the work will be able to start straight away it is likely that several iterations will be needed in order to find the optimal solution. A number of unknown will need to be investigated, including the issue of whether equilibrium chemistry is justified in the PDR and XDR region. Another issue is the sensitive dependance of the results on the specific dust (size) distribution in the PDR and XDR region. We will produce several models using the prescriptions of Birstiel, Klahr & Ercolano (2012) coupled to prescriptions for vertical mixing (e.g. ?????REF). This will allow us to assess, for what conditions, if any, FUV heating significantly affects the dispersal of discs and the formation/evolution of Type 1 transition discs.

The completion of this task will also depend on the completion of the tasks in project B2, thus it is likely that the final parameterisation will only be ready in year 2 of the first funding period.

At this point the MOCASSIN+ KROME code, enhanced by the initial reduced network from B2 (PI Caselli) will allow us to start producing the first chemical models of the wind and its atmosphere. We will be able to further investigate the nature of the broad-component of the neutral hydrogen emission, for which we have suggested a non-thermal origin coming from OH dissociation in the bound inner disc regions. The code chemical models will however most importantly form the basis to search for new wind diagnostics. In a joint effort with the B2 team we will produce synthetic observations that will be compared with available observations under the guidance of the A1 team (PI Testi) and out external collaborator Prof. van Dishoeck and Prof. Henning. This will guide the further development of the chemical model.

These activities will continue for the duration of the project, as the models are incrementally improved, by the addition of updated dust models, networks etc., until we are satisfied that a realistic synthetic spectrum can be delivered. This will allow us a quantitative comparison with the observations to finally constrain the models, allowing the determination of mass loss rates and wind profiles.

2.5.2.3 Month 18-36

The PI will work closely with Dr Picogna on the development and validation of a streamlined RT approach to be included in PLUTO for our means. This is likely necessary to estimate the value of the FUV field reaching different regions of the disc atmosphere, where the optical depth are not high enough to justify the use of a (grey) flux limited diffusion method (FLD).

We note that the PI is experienced in the development of efficient hybrid radiative transfer schemes for use in hydrodynamical simulation (e.g. Owen, Ercolano & Clarke 2012b). Finally, as MOCASSIN is able to solve the problem exactly for a given snapshot of the hydrodynamic calculation, we are in the rare position to be able to carefully check the validity of the new methods.

2.6 Data handling

A library of the hydrodynamical solutions in steady state (gas density and velocity) will be shared initially amongst the Research Unit members only and will be made available online on the public partition of the Research Unit server at the end of the first funding period.

The new temperature schemes will also be published in the relevant publications together with the mass loss profiles, which are important for the development of population synthesis models which include disc dispersal.

2.7 Other information

Not Relevant

2.8 Information on scientific and financial involvement of international cooperation partners

Not Relevant

3. Bibliography

[Text]

4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We require funding for one Postdoc to work at the LMU in the group of Prof. Ercolano. In case of an award Dr Picogna has agreed to take on the post. Dr Picogna is currently employed in the group of the PI and is performing preparatory work for the project. Dr Picogna's expertise in astrophysical fluid dynamics and his familiarity with the subject is of great advantage for the achievement of the aims of this project. Dr Picogna's contract ends in November 2017,

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Will be provided by the host institution

4.1.2.2 Travel Expenses

Total: 9900 Euro Justification : Each year one national trip (meeting of Astronomical Society, national meetings) and one international trip (conference, visit collaborators). During the course of the PhD 2 one week long visits to our main international collaborator, Dr J. Owen (currently at Princeton University, will move to Imperial College London in 2017).
Cost estimate:

- National trip: 5 overnight stays, train/airfare, conference fee; 1000 Euro (3000 over 3 years).
- International trip: 6 overnight stays, airfare, conference fee; 1500 Euro (4500 over 3 years).
- Visit to/from J. Owen: airfare, 6 overnight stay 1200 Euro (2400 for 2 visits)

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

Not Relevant

4.1.2.4 Other Costs

None

4.1.2.5 Project-related publication expenses

We request 770 Euro py (total 2250 Euro) for publication expenses.

4.1.3 Instrumentation

None

4.1.3.1 Equipment exceeding EUR 10,000

None

4.1.3.2 Major Instrumentation exceeding EUR 100,000

None

4.2 Module Temporary Position

Not Relevant

4.3 Module Replacement Funding

Not Relevant

4.4 Module Mercator Fellows

Not Relevant

4.5 Module Public Relations Funding

Not Relevant

5. Project requirements

5.1 Employment status information

Barbara Ercolano, Professor at the Ludwig-Maximilians-Universität München (permanent)

5.2 First-time proposal data

Not Relevant

5.3 Composition of the project group

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

This project will provide the radiation-hydrodynamic models of the wind which are needed by project B2 (PI: Prof. Caselli) for the chemical calculations and by project C2 (PI: Ercolano) for the dust entrainment. Project BI depends on input from project B2 (PI: Prof. Caselli) for the reduced network and on project A2 for observations. Specifically project A2 can provide insights on the emission properties of the irradiating stars.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

Dr James Owen (Princeton) will be heavily involved in the project. Dr Owen developed the original phoionisation models during his PhD project at the Institute of Astronomy in Cambridge, which was co-supervised by Prof. Ercolano. It is envisioned that Dr Owen will pay regular visit to our group to help with the development of the new models.

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

F. Niederhofer (STSci, USA); M. Hilker (ESO, Garching); N. Bastian (U. Liverpool, UK); M. Guarcello (U. Palermo, Italy); M. Tazzari (U. Cambridge, UK); A. Natta (Florence, Italy); R. Alexander (U. Leicester); D. Hubber (LMU); J. Dale (U. Hertfordshire, UK); C. Koepferl (LMU); I. Bonnell (U. St. Andrews, UK); A. McLeod (ESO, Garching); D. Boneberg (U. Cambridge, UK); R. Parker (U. Liverpool, UK); R. Wesson (UCL, London, UK); M. Barlow (UCL, London, UK); A. Glassgold (u. Berkeley, USA); C. Manara (ESA, Noordwjik, Netherlands); A. Danekhar (CfA, Harward, USA); Q. Parker (Sidney, Australia); S. Casassus (U. de Chile, Santiago, Chile); I. Pascucci (U. Arizona, USA); A. Bevan (UCL, London, UK).

5.5 Scientific equipment

The group of Prof. Ercolano has two own computer clusters comprising

- 2 CPU Intel Xeon X5650 (Westmere, beginning 2010, 2.66 GHz) 6 cores each 12 cores total (24 virtual) 74 GB ram.
- 4 CPU Intel Xeon E7-4850 (Ivy Bridge, beginning 2014, 2.30 GHz) 12 cores each 48 cores total (96 virtual) 660 GB ram.

Further computational power is provided through the C2PAP facility of the Excellence Cluster to which the group has guaranteed time. This comprises 126 nodes, each node with 2 CPU Intel Xeon E5-2680 (Sandy Bridge, beginning 2012, 2.7 GHz) 8 cores each 16 cores total (32 virtual) 64 GB ram. Note that while the future of the Excellence Cluster Universe is uncertain, the C2PAP facilities will be in any case supported by the LMU.

The Leibniz Rechnung Zentrum (LRZ) is also available to us, where still larger facilities are available with somewhat more constrained and longer queues.

5.6 Project-relevant interests in commercial enterprises

Not Relevant

5.7 Additional information

Not Relevant