Project C2:

Gone with the wind: Dust entrainment in photoevaporative winds

Authors:
PI: B. Ercolano (LMU)
Co-I: T. Birnstiel (LMU), C. Dullemond (Heidelberg)
Collaborations: James Owen (Princeton, USA), T. Henning (MPIA)

Requested positions: 1PhD student

Abstract:
The search for the smoking gun of disc dispersal via photoevaporative winds, leading to the formation of Type 1 TDs, has until now failed to identify suitable diagnostics. Quantitative spectroscopy of YSOs to search for blue-shifted emission lines produced in the wind relies on an accurate characterisation of the thermochemical properties of the winds. A central ingredients for the chemical calculations is the dust content of the wind as micron sized grains provide the dominant opacity channel in the far-ultraviolet. Furthermore small particles are important players in the temperature balance of the gas via the photoelectric process.

We will use realistic radiation-hydrodynamic models of photoevaporative winds coupled to dust evolution models for the underlying grain distribution in the disc, to calculate the dust entrainment in winds to feed to chemical models. The observability of the emission and scattering due to the dust grains in winds from edge-on discs, a potential new diagnostic, will be estimated for current and upcoming facilities (e.g. SPHERE, JWST) both for Herbig Ae stars and for their fainter T-Tauri counterparts.

1. State of the art and preliminary work

The dispersal of protoplanetary discs plays a crucial role in the planet formation process, and leads to the formation of Type 1 TDs. While photoevaporation from the central star has been proposed as the dominant disc-dispersal mechanism around low-mass stars (e.g. Clarke et 2001), to date the only direct evidence of a wind is the detection of blue-shifted line emission from some of the sources. The lines include [NeII] 12.8μm, [OI] 6300 and a number of other optical forbidden lines, which can be matched with more or less success by photoevaporation models (e.g. Hartigan, Edwards & Ghandour 1995; Alexander 2008; Rigliaco et al. 2013; Natta et al. 2014; Pascucci & Sterzik 2009; Schisano, Ercolano & Guedel 2010; Ercolano & Owen 2010, 2016, Simon et al. 2016). These lines however can only probe the wind on very local scales and they cannot be inverted to obtain mass loss rates, which are crucial to pin down the dominating mechanism which drives the disc photoevaporative wind (i.e. EUV, FUV or X-ray - or a combination). Different driving mechanism induce more or less vigorous mass loss at different disc radii, which can have dramatic effect on planet formation, both at the times of planetesimal assembly and for the later dynamical evolution of planet(esimal)s (e.g. Alexander & Pascucci 2012; Ercolano & Rosotti 2015, or the discussion in projects B1 and B2).

Projects B1 & B2 aim at identifying and using new spectroscopic diagnostics to quantitatively measure the mass loss rate and profile in disc winds. In order to achieve these aims a chemical model of the wind will be constructed in B2 using the wind structures from radiation-hydrodynamic calculations performed in B1. Chemistry is sensitively affected by the dust distribution in the wind and in the underlying disc atmosphere, but to date only rough estimates exist (e.g. Owen, Ercolano & Clarke

2011b; Hutchison et al. 2016ab). While the results of these works are not yet to the stage that they can be used in the chemical models, they demonstrate that a non-negligible population of small grains, which dominate the opacity in the FUV, are expected to be entrained in the winds.

Owen, Ercolano & Clarke (2011b) demonstrated that in the case of Herbig Ae/Be stars with an EUV-driven wind, the wind selectively entrains grains of different sizes at different radii resulting in a dust population that varies spatially and increases with height above the disc at radii larger than about 10 AU. This is a result of the streamlines topology, which extend roughly radially out. At near infrared wavelengths this variable grain population produces a 'wingnut' morphology which may have already been observed in the case of PDS 144N (Perrin et al. 2006). The work of Owen, Ercolano & Clarke (2011b) could not however reproduce the colour gradient of the observations, which show redder emission at larger heights above the disc. Owen, Ercolano & Clarke (2011b) suggested that the inconsistence may be due to the fact that the synthetic images are dominated by emission from the smallest grains entrained in the flow. Grain growth in the underlying disc, neglected in the Owen et al. (2011b) calculations, would reduce the population of small grains there and may provide a solution to the colour problem. The grain size evolution in the underlying disc needs to be taken into account in future simulations.

While it is currently not clear if the PDS 144N observations can be explained by dust entrainment in a photoevaporative wind, the work of Owen, Ercolano & Clarke (2011b) has clearly demonstrated that a significant amount of small grains (which dominate the opacity in the FUV) do populate disc winds, hence playing an important part in the chemistry there and at the base of the flow.

More recently Hutchison et al. (2016ab) investigated the question of dust entrainment in protoplanetary discs using smoothed particle hydrodynamics (SPH). While their models are very idealised (non-rotating, plane-parallel discs), their simulations seem to support most of the conclusions reported in the semi-analytical work of Owen, Ercolano & Clarke (2011b). The Hutschison et al. models also only consider an a EUV-driven wind, in order to simplify the calculations.

1.1 Dust-entrainment in winds: two modelling strategies

In this section the two approaches to model dust-entrainment in winds mentioned above are described in more detail. The limitations of both approaches are also discussed, thus highlighting the knowledge gap that our project is aiming to fill.

1.1.1 Analytical approach

Owen, Ercolano & Clarke (2011b) post-processed radiation-hydrodynamical simulations of photoevaporating disc winds around Herbig Ae/Be stars in order to study the distribution and observational appearance of dust grains entrained in the wind. Their approach involved three steps: (i) (radiation)-hydrodynamical calculations of the photoevaporative wind; (ii) calculation of the dust profile distribution in the wind; (iii) radiative transfer calculation of the dust distribution to infer the observational appearance.

As the work of Owen, Ercolano & Clarke (2011b) was motivated by the observations of several edge-on discs around Herbig stars, which showed extended emission above and below their midplane at NIR wavelengths (e.g. Padgett et al. 1999, Perrin et al. 2006), these authors focussed in step (i) on EUV-driven winds (e.g. Hollenbach et al. 1994; Font et al. 2004; Alexander, Clarke & Pringle 2006a,b). Indeed Herbig stars have generally a much lower X-ray luminosity relative to their bolometric luminosity, compared to T-Tauri stars, raising questions on what the driving radiation may be for these intermediate mass stars. For that reason Owen, Ercolano & Clarke (2011b) chose to adopt the hydrodynamic EUV wind solution of Font et al. (2004), which is simple and scalable, hence allowing them to investigate a wider range of parameter space. As we will see in Section 2, this option is not suitable for T-Tauri stars we wish to model here, where the X-ray photoevaporation model needs to be

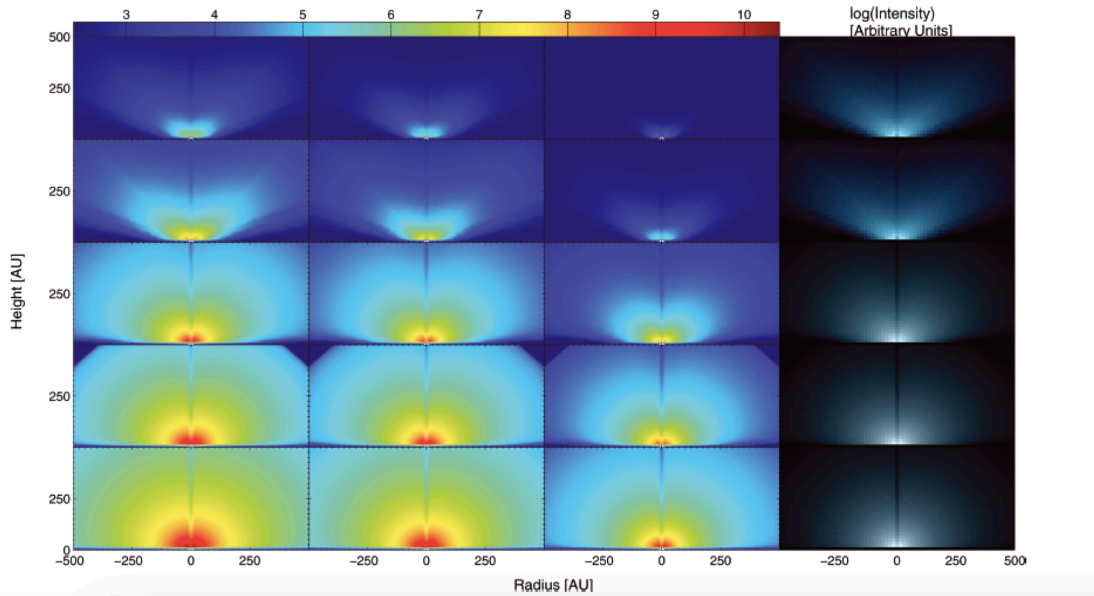

Figure 1: Image from Owen, Ercolano & Clarke (2011b): Synthetic images for disc models with irradiating fluxes $\phi = 1e41....1e45 phot/sec$, the **far left-hand column** shows the image in the H band, the **next column** displays the K band and the **other next column** displays the L band. The **far right-hand column** displays a red green blue composite image (L,K and H bands, respectively). The images are individually scaled so that there is a 5 dex spread between the brightest pixel and the darkest. All images assume that the disc is edge-on, therefore the stellar emission is blocked out by the presence of the optically thick disc.

considered. X-ray driven photoevaporative winds, are shown to be two orders of magnitude stronger than EUV-winds around T-Tauri stars.

In step (ii) Owen, Ercolano & Clarke (2011b) calculated streamlines from the base of the flow to the edge of their grid from the solutions obtained in step (i). Along each of the streamlines the balance between the drag force, gravity and the centrifugal force was then calculated for a given grain size: a positive net force was interpreted as grains of that size being entrained in the flow from that location.

The density distribution of dust grains in the wind was then calculated and post-processed by means of radiative transfer in step (iii) . Figure 1 shows the synthetic images obtained from the models of Owen, Ercolano & Clarke (2011b) in L,K & H band and composite, which were then compared with the observations of Perrin et al. (2006).

While the calculations of Owen, Ercolano & Clarke show that indeed a significant amount of small grains can be expected in photoevaporative winds, they present however some serious limitations that make them unsuitable for application to our Research Unit tasks. First of all, these calculations are limited to the EUV-case only. The X-ray photoevaporation case, which is likely dominant amongst T-Tauri stars, is completely different and significantly more complex than the EUV case.

Another important shortcoming of Owen, Ercolano & Clarke (2011b) is that they do not account for dust evolution in the underlying disc. An MRN (Mathis, Rumpl, Nordsieck 1977) size distribution with standard gas-to-dust ratio of 100 is assumed everywhere in the disc. The resulting dust density and size distribution in the wind is thus necessarily incorrect. Given the central role played by dust grains for the chemistry (see project B2), our project will couple dust evolution in the underlying disc to the wind entrainment problem for the X-ray driven winds around T-Tauri stars.

1.1.2 Numerical approaches

The dynamics of dust grains in protoplanetary discs can be studied either by directly integrating the orbits of a large number of dust 'super-particles' (that sample the local properties of the dust population) or by solving the collisionless Boltzmann equation for the particle distribution function. For a population of very small (tightly coupled with the gas) dust particles, the Boltzmann equation can be reduced to the zero pressure fluid equation (Cuzzi et al. 1993, Garaud et al. 2004). This 'two-fluid' approach has been used to study planet-disc interactions (e.g. Paardekooper & Mellema 2004, 2006; Zhu et al. 2012). This is however limited to a single population of small particles, it cannot account for the full velocity distribution of the grains at a single location, and it is not able to capture strong density gradients. The particle approach has the great advantage to follow the evolution of solid particles with different physical properties, perfectly recovering the dust dynamics in the limit where the grains are decoupled from the gas (Youdin & Johansen 2007; Miniati 2010; Bai & Stone 2010). This method has also been applied successfully to the study of planet disc interaction adopting both SPH and grid-based codes (Fouchet et al. 2007, 2010; Ayliffe et al. 2012; Lyra et al. 2009; Zhu et al. 2014). Grid codes are generally preferred because they do not introduce a large artificial viscosity that can affect the evolution of low-mass planets. Moreover, the accuracy needed to properly model the evolution of the gas and dust component in a protoplanetary discs is strongly dependent on the choice of the grid geometry (Lyra et al. 2009; de Val-Borro et al. 2007), requiring more computational effort in a cartesian grid than in a cylindrical or spherical one.

Dr. Picogna, who is currently employed as a postdoc in the group of PI Ercolano, has implemented a population of dust particles in the modern grid-based code PLUTO (Mignone et al. 2012) that can evolve both in a cylindrical and spherical coordinate system (Picogna, Stoll & Kley, in prep.). This approach is thus ideal to study the evolution of different dust particle populations in protoplanetary discs. As detailed in the next section, this method, coupled with the photoevaporation model implemented in PLUTO, will be adopted to self-consistently model dust particles entrained into the wind from the disc atmosphere for a number of selected cases.

In their recent work of Hutchison et al. (2016a,b) used a new algorithm to treat a wind in an SPH code. The wind is treated using unequal-mass, one-fluid SPH. Using new techniques developed by the authors, they are able to simulate two-fluid dynamics in highly stratified atmospheres. The work currently represents only a proof of concept, suggesting, however, that these novel techniques may in the future be applied to study interesting aspects of gas and dust dynamics in the wind. At present, however, the models are very idealised, approximating discs and winds by a thin, non-rotating, plane-parallel atmosphere. This technique is thus not yet mature to be used for the purposes of our project.

1.2 Project-related publications

Birnstiel, T.; Dullemond, C.P. & Brauer, F.: *Gas and dust evolution in protoplanetary disks*, 2010, A&A 513, 79. In this paper we present the basic code for the evolution of the disk and the dust. The latter follows the dust coagulation, fragmentation, settling and radial drift of the dust.

Birnstiel, T.; Klahr, H. & **Ercolano, B.**: *A simple model for the evolution of the dust population in protoplanetary disks*, 2012, A&A 539, 148. In this model the flow of pebbles from the outer disk regions into the inner planet forming disk regions is studied, and an easy to use model derived.

Birnstiel, T.; Andrews, S.; Pinilla, P. & Kama, M.: *Dust Evolution Can Produce Scattered Light Gaps in Protoplanetary Disks*, 2015, ApJL 813, L14. Here we applied the vertical steady state settling mixing distribution to calculate the observational appearance of simulated disks.

Ercolano, B.; Drake, J.; Raymond, J. C.; Clarke, C. C.: *X-Ray-Irradiated Protoplanetary Disk Atmospheres. I. Predicted Emission-Line Spectrum and Photoevaporation*, 2008, ApJ 688, 398. We present mocassin two-dimensional photoionization and dust radiative transfer models of a prototypical T Tauri disk irradiated by X-rays from the young pre-main-sequence star. In this work a first estimate of X-ray photoevaporation rates is given, hinting at the relevance of this process for disc dispersal

Ercolano, B.; Clarke, C. C.: Drake, J.; *X-Ray Irradiated Protoplanetary Disk Atmospheres. II. Predictions from Models in Hydrostatic Equilibrium*, 2009, ApJ 699, 1639. In this follow-up paper we take into account the response of the disc structure to the X-ray heating and demonstrate that even in this case the X-ray photoevaporation rates remain substantial. A hydrostatic solution is reached iteratively with the full photoionisation problem.

Owen, J. E.; **Ercolano, B.**; Clarke, C. J.; Alexander, R. D. *Radiation-hydrodynamic models of X-ray and EUV photoevaporating protoplanetary discs*, 2010, MNRAS, 401, 1415. Starting from the hydrostatic solutions of Ercolano et al 2009, we perform the first radiation-hydrodynamic solution of an X-ray irradiated disc. Robust mass-loss-rates and profiles are calculated for this model, suggesting that X-ray drive the dispersal of discs.

Owen J., **Ercolano B.**, Clarke C. *Protoplanetary disc evolution and dispersal: the implications of X-ray photoevaporation*, 2011a, MNRAS, 412, 13. We explore the role of X-ray photoevaporation in the evolution and dispersal of viscously evolving T Tauri discs. Our models confirm that X-rays play a dominant role in the evolution and dispersal of protoplanetary discs giving rise to the observed diverse population of transition discs, including some of those with massive outer discs, some of those with gas in their inner holes and some of those with detectable accretion signatures.

Owen J., **Ercolano B.**, Clarke C. *The imprint of photoevaporation on edge-on discs*, 2011b, MNRAS, 411, 4103. We perform hydrodynamic and radiative transfer calculations of a photoevaporating disc around a Herbig Ae/Be star to determine the evolution and observational impact of dust entrained in the wind. We find that the wind selectively entrains grains of different sizes at different radii resulting in a dust population that varies spatially and increases with height above the midplane.

Owen J., Clarke & **Ercolano B.** *On the theory of disc photoevaporation* 2012, MNRAS, 422, 1880. We derive analytical scaling relations and derive estimates for the total mass-loss rates, as well as discussing the existence of similarity solutions for flows from primordial and transition discs. In this paper we catch a first glimpse at a new process for the clearing of the very last stages, which we name "thermal sweeping".

Ercolano B., Owen J. *Blueshifted [O I] lines from protoplanetary discs: the smoking gun of X-ray photoevaporation*, 2016, MNRAS 460. 3472 We produce new synthetic observations of a particularly promising diagnostic, and demonstrate that the observations available at the time (before Simon et al. 2016) are consistent with the photoevaporation model. We show however that this line cannot be used to measure mass-loss-rates.

2. Objectives and work programme

2.1 Anticipated total duration of the project

36 months

2.2 Objectives

In this project we aim to determine the dust content and size distribution of photoevaporative winds for a range of stellar, disc and wind parameters, using realistic descriptions for grain evolution in the underlying disc.

This will allow us to :

1. Build a dust model for photoevaporative winds to be used in astrochemistry and radiative transfer calculations (see B2).
2. Estimate the observability and observation characteristics of the dust phase in photoevaporative winds.

2.3 Work programme including proposed research methods

In this project we will first use the semi-analytical approach described in Section 1.1.1 coupled to models for the evolution of dust grains in the disc in order to efficiently produce dust entrainment models for the complete set of X-ray photoevaporation wind solutions calculated in project B1. The dust models will then be passed on to project B2 (chemical models), incrementally as they are calculated.

There are several reasons for choosing the semi-analytical approach over fully numerical approaches (SPH or grid-based). First of all, semi-analytical approaches are much more efficient for our aims. We will make use snapshots from the hydrodynamical calculations, since, to first order, the grain entrainment problem can be decoupled from the photoevaporation problem. Indeed dust grains entrained in the wind do now provide tangible extinction at X-ray frequencies, hence the wind structures and rates are not sensitive to the dust distribution in the wind. The dust entrainment calculation can thus be performed by post-processing snapshots of the radiation-hydrodynamic calculations, allowing us to use the same wind solution and changing (e.g.) the underlying dust distribution in the disc, according to different models and prescriptions.

It is perhaps worth mentioning that the dust evolution in the underlying disc is however strongly coupled to the evolution of the gas in the disc. A full radiation-hydrodynamic simulation of the gas and dust which also simultaneously solves the dust coagulation and drift is however beyond what is currently feasible. It is however possible to perform a gas radiation hydrodynamics calculation which includes dust particles, not accounting for coagulation (e.g. Picogna, Stoll & Kley , in preparation).

If time allows, we will perform a number of such (expensive) calculations to compare with the semi-analytical ones. This is particularly important for transition disc models, where the dust may be pushed back away from the inner edge of the disc due to the pressure gradients in the gas, thus resulting in a lower dust content in TD winds, compared to full discs. In any case, a more comprehensive set of these simulations will be performed during the second funding period of the Research Unit.

2.3.1 Grain sizes and abundances at the base of the wind

One key element of this project is to investigate the impact of the underlying grain population on the population of grains entrained in photoevaporative winds. To this end we will use the state of the art coagulation code from Birnstiel et al. (2010) which solves for the evolution of the particle distribution due to coagulation, fragmentation, and erosion, as well as radial transport by drift, mixing, and gas advection. The resulting particle size distribution $\Sigma_d(t, r, a)$ is then a function of distance to the star r, particle size a, and time t. Treating the growth in a vertically averaged way (i.e. using surface densities instead of volume densities) is generally a good approximation since vertical settling and mixing time scales are short for growing particles. However, for this project, the vertical distribution of particle sizes is important as it determines the sizes and abundances of particles at the base of the photoevaporative flow.

At the beginning of the project, we will use vertical distributions of particles that are in a steady state between mixing and settling, such as derived by Fromang & Nelson (2009). These are simple analytical equations, which need to be numerically integrated for each particle size. This technique is already available and has been used for calculating the observational appearance of simulated disks e.g. in Birnstiel et al. (2015) and many other works. This should give a good first representation of the particles that are present at the base of the flow.

At a later point, these prescriptions can be updated with a more sophisticated treatment of coagulation and transport processes: at high dust-to-gas ratios small grains can be “trapped” closer to the mid-plane due to frequent collisions with other particles (Krijt & Ciesla 2016). When photoevaporation has preferentially depleted the gas, thus raising the dust-to-gas ratio in the disk, this effect could potentially affect the amount of small dust grains that are mixed up to the base of the photoevaporative flow. The results of Krijt & Ciesla (2016) can be used to estimate this effect. Some time during the second year of this project, we expect the ERC group of T. Birnstiel to have a working 2D dust coagulation and transport model which will allow us to check for differences between the earlier approaches (steady state distributions) and models that take the time evolution and collisional processes into account.

2.3.2 Research Tools and Inputs

For this project we will need the following tools:

1. Photoevaporative wind solutions for EUV-driven models for T-Tauri and Herbig stars. These are easily computable using the models that are described in the literature (e.g., Font et al. 2004).

2. Photoevaporative wind solutions for X-ray photoevaporated models. These will be provided from project B1.

3. One-dimensional dust growth models. These codes are published and available within the group: simulation code of Birnstiel et al. (2010) and the parameterized model of Birnstiel et al. (2012). The one dimensional results will be coupled to prescriptions of vertical mixing (Fromang & Nelson 2009, e.g.)

4. Two-dimensional dust evolution results/parameterisation from the ERC-funded projects of Dr. Birnstiel.

5. A 3D radiative transfer code to post-postprocess the wind models with the calculated grain populations. For this we can use the streamlined version of the MOCASSIN code developed by the PI (see description below) and/or use of the RadMC3D code developed and maintained by Prof. Dullemond.

2.3.3 Research Plan

The work proposed here will be carried out by a PhD student supervised by Prof. Ercolano (LMU) with the help of Dr. Birnstiel (LMU), who will advice, respectively, on the dust entrainment calculations and the coupling with the dust evolution models for the underlying disc.

The project will proceed in stages of increasing complexity. We will start by setting up a framework that can be benchmarked against available calculations and progressively adding new elements, as they become available from other projects. The plan has been designed to fit a PhD student, who will have the opportunity to develop a new theoretical model as well as acquainting her/himself with standard numerical techniques (e.g. radiation-hydrodynamics, dust evolution models, radiative transfer).

The most important science product from this project is the set of grain models developed for the X-ray driven wind. These are needed by project B2 for the chemical calculations, as the dust grains dominating the opacities in the FUV are not equally distributed in the wind (see e.g. Owen, Ercolano & Clarke, 2011b, Hutchison et al. 2016ab) and they thus affect the chemistry in the wind differently in different parts.

2.3.3.1 Preparatory Work

The methodology described in Owen, Ercolano & Clarke (2011b), has been used in the group of the PI Ercolano to develop a suit of codes which take the gas density and velocity of the EUV-only wind and the stellar irradiation spectrum as an input and calculate the dust density and size distribution in the wind.

The resulting codes are the product of first a bachelor and then a master student project in the group of PI Ercolano. The aim of the bachelor project performed by George Dadunashvilli in 2013 and of the master project performed by Denis Mehmedov in 2014, was to asses the role played by dust growth in the underlying disc on the appearance of the wind in the case of the EUV-only driven wind from the Herbig star studied by Owen, Ercolano & Clarke (2011b).

The projects were motivated by the failure of the Owen, Ercolano & Clarke (2011b) models in reproducing the colour gradient in the observations of PDS 144N (Perrin et al. 2006), which show redder emission at larger heights above the disc.

The main results of the two projects can be briefly summarised as follows. In the case of an EUV-only wind, the removal of small grains from the disc atmosphere due to grain growth produces an overall reduction in the total dust density in the wind. This can be seen in Figure 2, where the dust density distribution in the wind is compared for the case of an underlying disc grain size distribution following a standard MRN (Mathis, Rumpl & Nordseick 1977) and for a truncated MRN. The colours of the wind are also affected by the removal of small grains in the disc, but not enough to reproduce the observations. A comparison of different calculations for different grain size cut-offs are shown in Figure 3.

There are a number of problems with these preliminary results however. First of all a full exploration of the parameter space, even if only for the EUV-only case is beyond the scope of bachelor or even master projects. This is one of the reason why these results have yet to be published. Furthermore an unrealistically simplified approach to including the effects of grain growth was used. Simply a cut-off was applied to the minimum grain size in the MRN distribution of the underlying disc. This led to the fact that we have been limited to a maximum cut-off of 0.73*mu*m. A cut-off at larger sizes would have led to a virtually dust-free wind. This is unrealistic since the growth of grains in a more realistic

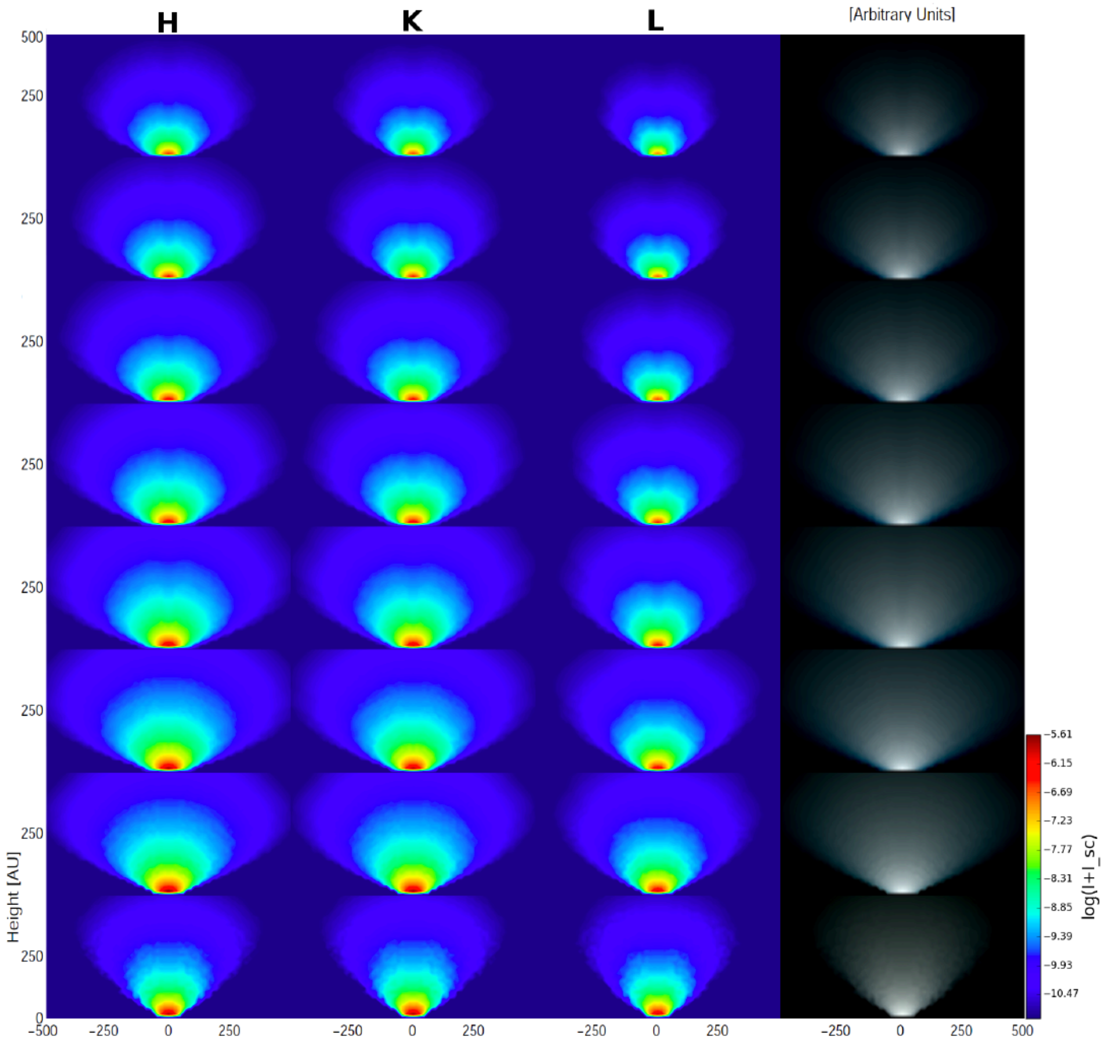

Figure 2: Effect of sequential truncation of MRN on the image. **Columns, from left to right respectivley:** H: (1.5 - 1.8)μm, K: (2 - 2.4)μm, L: (3 - 4)μm. Rows from top to bottom correspond to MRN in the disk with respectively: a_{min} = 5, 10, 20, 42.4, 86, 170, 360, 730 nm and a_{max} = 1mm. **First three columns of all rows** are normalized such that there are 5 dex between the brightest value in the L band of all images, representing the white pixel and the black pixel. Figure taken from the LMU Master Thesis of Denis Mehmedov, 2015.

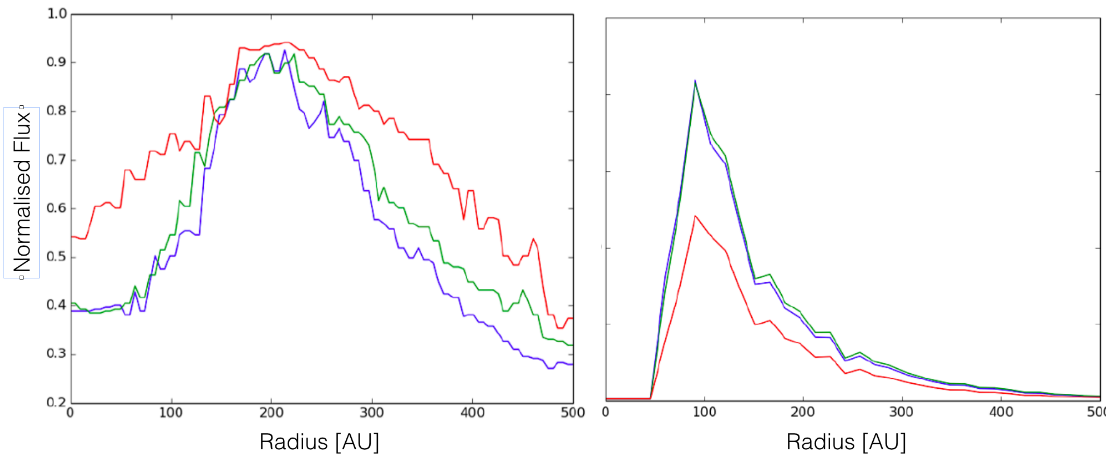

Figure 3: **Left Panel:** Color plot of the slice at 100AU in the observational images extracted from Perrin and Graham (2006). **Right Panel:** The same for out simulation with the maximum truncation of the MRN (a_{min}=730nm). Figure taken from the LMU Master Thesis of Denis Mehmedov, 2015.

coagulation model leads to a larger population (by number) of a few micron-size grains compared to a standard MRN which is truncated at say 1*mu*.

Nevertheless, the legacy of these projects is a suite of codes, which were benchmarked in detail, and result now much improved compared to the Owen, Clarke & Ercolano (2011b) tools. These can be used as a starting point and upgraded by the PhD student employed for the project.

2.3.3.2 Months 1-12

The student will start by producing wind solution for the EUV case from the work of Font et al. (2004), which may be applicable to Herbig stars. For that she/he will use the standard version of the PLUTO code (Mignone et al. 2007, 2012) in two-dimensional mode. Note that no additional column density/Stroemgren radius calculations need to be used in order to implement the Font et al. (2004) solutions for EUV winds. This solution simply treats the wind as an isothermal gas with sound speed, c_s = 10 km s^{-1}. The number density at the base of the wind is also fixed and is a simple function of radius, mass of the central star, gas sound speed and ionising stellar flux (Font et al. 2008, Alexander 2009, Hollenbach et al. 2004). We will be able to validate our solutions with those in the literature, which is an important step, particularly in a project led by a PhD student.

The student will then proceed to calculate the dust distribution in the wind, under simplifying assumptions for the underlying dust distribution in the disc as in Owen et al. (2011). In brief, streamlines from the base of the flow to the edge of the grid will be computed and along each of them, the force balance between the drag force, gravity and the centrifugal force will be calculated. A positive net force on a grain along the streamline will indicate that the grain is entrained.

Once dust abundance and size distributions have been obtained for the wind, radiative transfer calculations will be performed to produce synthetic continuum observations at several disc inclinations. These first models will be benchmarked against the solutions of Owen et al. (2011). Note that we have developed a streamlined version of our MOCASSIN code which was used to produce the images in Owen et al. (2011), as well as in the subsequent bachelor and master thesis projects. However the RADMC-3D code developed by Prof. Dullemond (co-speaker to the Research Unit) is also available to us for comparison.

After the benchmarking tests, we will be sure that we have developed a solid framework which can now be applied, for the first time, to the calculation of the dust component entrained in an X-ray driven photoevaporative wind. The wind solutions of Owen et al. (2010, 2011, 2012) and Ercolano & Owen

(2016) are readily available and they could provide a starting point, until new wind solutions become available form project B1. This may however not be necessary as the new wind models for the X-ray case are already being calculated by Dr. Picogna, who is employed to do the preparatory work for project B1. It is therefore likely that an initial set of high resolutions new X-ray wind solution may already be available to the student right from the start of project C2.

As the first dust models for the X-ray driven wind become available they will be immediately passed on to project B2 (Astrochemistry), for inclusion in the chemical models to be then updated when the new models including dust evolution in the disc become available (see next section).

We will perform new radiative transfer calculations of the dusty X-ray driven wind to produce synthetic continuum observations and provide a first estimate of the observability of such winds with current/future instrumentations. Our results may motivate observational campaigns led by collaborators (e.g. the group of Prof. Henning), the outcome of which, however does not influence the success of the research aims of our projects. In

2.3.3.3 Months 13-24

At this point we will be in a position to significantly improve on this work by considering more realistic grain abundances and size distributions for the underlying disc.

We will first couple the grain entrainment calculations to simple prescriptions of dust evolution (e.g., Birnstiel et al. 2012) obtained from the one-dimensional models of Birnstiel et al. (2010). The one dimensional models describe the evolution of dust that is mostly in the mid-plane, i.e. well below the base of the wind, where the grains may be entrained from. The Birstiel, Klahr & Ercolano (2012) prescriptions will then need to be coupled to vertical mixing prescriptions (Fromang & Nelson 2009) in order to estimate the grain distributions at the wind-launching location, obtained from the hydro simulations. While this is not optimal, it is the standard approach used in this field as a two-dimensional model of dust evolution is still lacking. As an example the observational appearance of simulated disks is generally calculated in this way (Birnstiel et al. 2015, e.g.).

Complementary to this project the ERC-funded team led by Dr. Birnstiel aims to develop new two-dimensional (both radius-height and radius-azimuth) dust evolution models. When these new models become available, the student will work closely with Dr. Birnstiel to include elements of these new results in our calculations.

As the first new models which account for grain evolution in the underlying disc become available for a few selected cases, they will be implemented in the astrochemistry models of project B2. In collaboration with the postdoc employed for project B2, we will then compare the resulting chemical models with those obtained in the previous year, which assumed a standard MRN distribution for the underlying disc. This will allow us to estimate the effects due to the coupling of grain evolution and grain entrainment in the wind on the chemical abundance in the wind and disc atmosphere. This step is important to establish to what degree of complexity this coupling should be performed in order to ensure accurate results.

2.3.3.4 Months 25-36

In this last year of the first funding period the whole machinery will be in place. We will now be able to apply it to a wide parameter space of disc winds, producing sets of dust models to be passed on to project B2 for the optimised chemical calculations.

At this stage it will also be interesting to connect with project C1, where models of discs with dust traps are to be developed. The question to be asked is “What is the effect of dust traps in the underlying disc on the grain entrainment? Can one expect signatures of this process to be observed either in the continuum emission in the wind or in the molecular lines observations?”

We will perform comprehensive dust radiative transfer calculations of the obtained structures (with and without dust traps) to compare with available observations or to make more detailed observability predictions, which may further guide future observing proposals. We will join forces with expert collaborators on scattered light observations (e.g. Prof. Henning, Prof. Dullemond) to plan new proposals, however we stress that failure to obtain new observations as well as eventual non-detections do not preclude the main aim of this project to be achieved, i.e. the development of dust models and dust distributions in photoevaporative winds.

Furthermore, as detailed in a previous section, we plan to compare and contrast the efficiency of dust entrainment for discs at different evolutionary stages. In order to do that we will use grids of TD discs from model B1 with cavities of various sizes, where the streamline topologies are different from those of full discs.

If time allows, the student will collaborate with the postdoc employed for project B1 to produce full hydrodynamical simulations of disc winds, where the dust component in the disc and wind is treated as particles (e.g. Picogna & Kley 2016). As we discussed in the previous sections of this proposal, these calculations are computationally expensive and therefore we will only be able to perform a limited number of them. Nevertheless they may be useful as a piecewise comparison to the simpler methods previously developed by the student in the project.

A more comprehensive set of simulations, performed via the semi-analytical and (for a smaller sample) the numerical method, will be performed in the second funding period. These will also include photoevaporating discs with gaps opened by giant planets (e.g. Rosotti, Ercolano et al. 2013, 2015), for which the models developed in project D1 will provide the starting conditions.

2.4 Data handling

The model data-grids will be made available on the Research Unit dedicated server for use within the team. Furthermore we will provide a set of diagnostic models to guide observers in the wider community, which will be placed on the public partition of the server. This public data will include sets containing the full size distribution at every 2D point, as well as sets of the mean/minimum/maximum grain sizes (the mean averaged in different ways), as well as synthesised images in different bands which can be directly compared to observations.

2.5 Other information

Not Relevant

2.6 Information on scientific and financial involvement of international cooperation partners

Not Relevant

3. Bibliography

Kees to Barbara: Shall I convert all your references to bibtex for you? Then we get a same style in all projects and it will be easier to handle. BARBARA TO KEES: YES PLEASEEEEE

Birnstiel, T., Andrews, S. M., Pinilla, P., & Kama, M. 2015, ApJ, 813, L14
Birnstiel, T., Dullemond, C. P., & Brauer, F. 2010, A&A, 513, A79
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Font, A. S., McCarthy, I. G., Johnstone, D., & Ballantyne, D. R. 2004, ApJ, 607, 890
Fromang, S. & Nelson, R. P. 2009, A&A, 496, 597

Krijt, S. & Ciesla, F. J. 2016, ApJ, 822, 111
Owen, J. E., Ercolano, B., & Clarke, C. J. 2011, MNRAS, 411, 1104

4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We require funding for one PhD student to be supervised at the LMU by Prof. Ercolano.

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 €
Justification: Each year one national trip (e.g., meeting of Astronomical Society, national meetings) and one international trip (conference, visit to 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 € (3000 over 3 years).
- International trip: 6 overnight stays, airfare, conference fee; 1500 € (4500 over 3 years).
- Visit to/from J. Owen: airfare, 6 overnight stay 1200 € (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 750 €/year (total 2250 €) 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

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

The project will use the wind models calculated in project B1 (PI Ercolano) and then feed back the results to project B2 (PI Caselli, Ercolano), where a chemical model of the wind and atmosphere will be developed. Dr. Birnstiel will provide guidance on the implementation of existing and new dust evolution models and, in the one-dimensional case, also helping us to link them to vertical mixing prescriptions. Models for 2d dust evolution of the underlying disc will be provided by the ERC-funded group of Dr Birnstiel. In the third year of the Research Unit we will connect with project C1 to use the dust distributions in the underlying discs. Stellar properties to guide the models will be obtained with the help of the team from project A2 (PI Preibisch). Observational constraints will be obtained in collaboration with experts working on project A1 (PI Testi) and our external collaborators Prof. Henning and Prof. van Dishoeck.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

Dr. James Owen, currently at Princeton University, from 2017 at Imperial College London, has performed the original semi-analytical calculations of dust-entrainment in the wind together with the PI of this project (Owen, Ercolano & Clarke, 2011b). He is also an expert in radiation-hydrodynamics models of photoevaporating winds (e.g. Owen, Ercolano et al. 2010, 2011a, 2012) and is expected to pay frequent visit to Munich to actively participate in our project.

We also plan to use the 2D dust evolution models which will be constructed within the ERC- funded group of Dr. Birnstiel, which will run parallel to the Research Unit.

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

R. Alexander (U. Leicester), S. Andrews (Harvard, USA), X. Bai (Harvard, USA), A. Banzatti (STScI Baltimore, USA), M. Barlow (UCL, London, UK), N. Bastian (U. Liverpool, UK), M. Benisty (IPAG Grenoble, FRA), A. Bevan (UCL, London, UK).D. Boneberg (U. Cambridge, UK), I. Bonnell (U. St. Andrews, UK), J. Carpenter (California Institute of Technology), C. Carrasco-González (UNAM, MEX),

S. Casassus (U. de Chile, Santiago, Chile), P. Cazzoletti (MPE, DEU), J. Dale (U. Hertfordshire, UK), A. Danekhar (CfA, Harward, USA), C. Dominik (Univ. Amsterdam, NLD), C. Dullemond (Univ. Heidelberg, DEU), A. Dutrey (Univ. Bordeaux, FRA), M. Fang (Purple Mountain Obs., CHN), M. Flock (JPL, USA), A. Glassgold (U. Berkeley, USA), U. Gorti (SETI Institute, USA), M. Guarcello (U. Palermo, Italy), S. Guilloteau (Univ. Bordeaux, FRA), T. Henning (MPIA, DEU), M. Hilker (ESO, Garching), M. Hogerheijde (Leiden Observatory, NLD), D. Hubber (LMU), A. Isella (Rice Univ., USA), A. Johansen (Lund Univ., SWE), M. Kama (Leiden Observatory, NLD), A. Kataoka (Univ. Heidelberg, DEU), H. Klahr (MPIA, DEU), C. Koepferl (LMU), H. Linz (MPIA, DEU), C. Manara (ESA, Noordwjik, Netherlands), A. McLeod (ESO, Garching), R. Murray-Clay (UCSB, USA), A. Natta (DIAS, IRL), F. Niederhofer (STSci, USA), R. Parker (U. Liverpool, UK), Q. Parker (Sidney, Australia), I. Pascucci (U. Arizona, USA), P. Pinilla (Leiden Observatory, NLD), A. Piso (Harvard, USA), A. Pohl (MPIA, DEU), L. Pérez (MPIfR, DEU), L. Ricci (Harvard, USA), V. Roccatagliata (LMU, DEU), K. Rosenfeld (Harvard, USA), D. Semenov (MPIA, DEU), M. Tazzari (U. Cambridge, UK), R. Teague (MPIA, DEU), L. Testi (ESO), C. Walsh (Leiden Observatory, NLD), R. Wesson (UCL, London, UK), D. Wilner (Harvard, USA), Z. Zhu (Princeton U., USA), M. de Juan Ovelar (Liverpool Univ., GBR), R. van Boekel (MPIA, DEU), E. van Dishoeck (Leiden Observatory, NLD), N. van der Marel (Leiden Observatory, NLD), K. Öberg (Harvard, USA),

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.