X-ray Radiative Transfer in Protoplanetary Disks with ProDiMo

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Introduction

X-ray emission is a common property of YSOs. T-Tauri stars show X-ray luminosities up to 10^{31} erg s^{-1} but also Herbig Ae/Be stars can have moderate X-ray emission in the range of 10^{28} to 10^{30} erg s^{-1}. We are investigating the impact of X-ray radiation on the thermal and chemical structure of protoplanetary discs around these YSOs.
Therefore we have added a new **X-ray radiative transfer (RT) module** to the radiation thermo-chemical code ProDiMo (PROtoplanetary DIsc MOdel) extending the existing implementation of X-ray chemistry by Aresu et al. (2011).
This new RT module includes X-ray scattering (gas and dust) and a treatment for possible X-ray background fields. Further, we added a new set of FUV-photoreactions for the X-ray chemistry module as X-ray ionisation produces a secondary FUV radiation field.
We present our methods and discuss first results where we focus on the impact of the mentioned X-ray physical processes on the chemistry of the disk and on the observables like sub-mm spectral lines.

The X-ray Radiative Transfer (RT) Module

- **X-ray Scattering**
  For the X-ray scattering cross-sections (Compton and Rayleigh) we use the open source library *xraylib* (Schoonjans et al., 2011). The anisotropic behaviour of Compton scattering is treated via an approximation by reducing the isotropic scattering cross-section by a factor $1-g$, where g is the anisotropic scattering factor. As ionisation due to X-rays changes the gas opacities we apply a global iteration scheme involving the RT and the chemistry.
- **X-ray Dust Opacities**
  We use the method of Draine (2003) (Kramers-Kronig relation) to calculate X-ray dust opacities (absorption and scattering) for various dust compositions by using the available optical constants for the UV to mm range and gas phase cross-sections for the X-ray range. See Fig. 1 for an example.

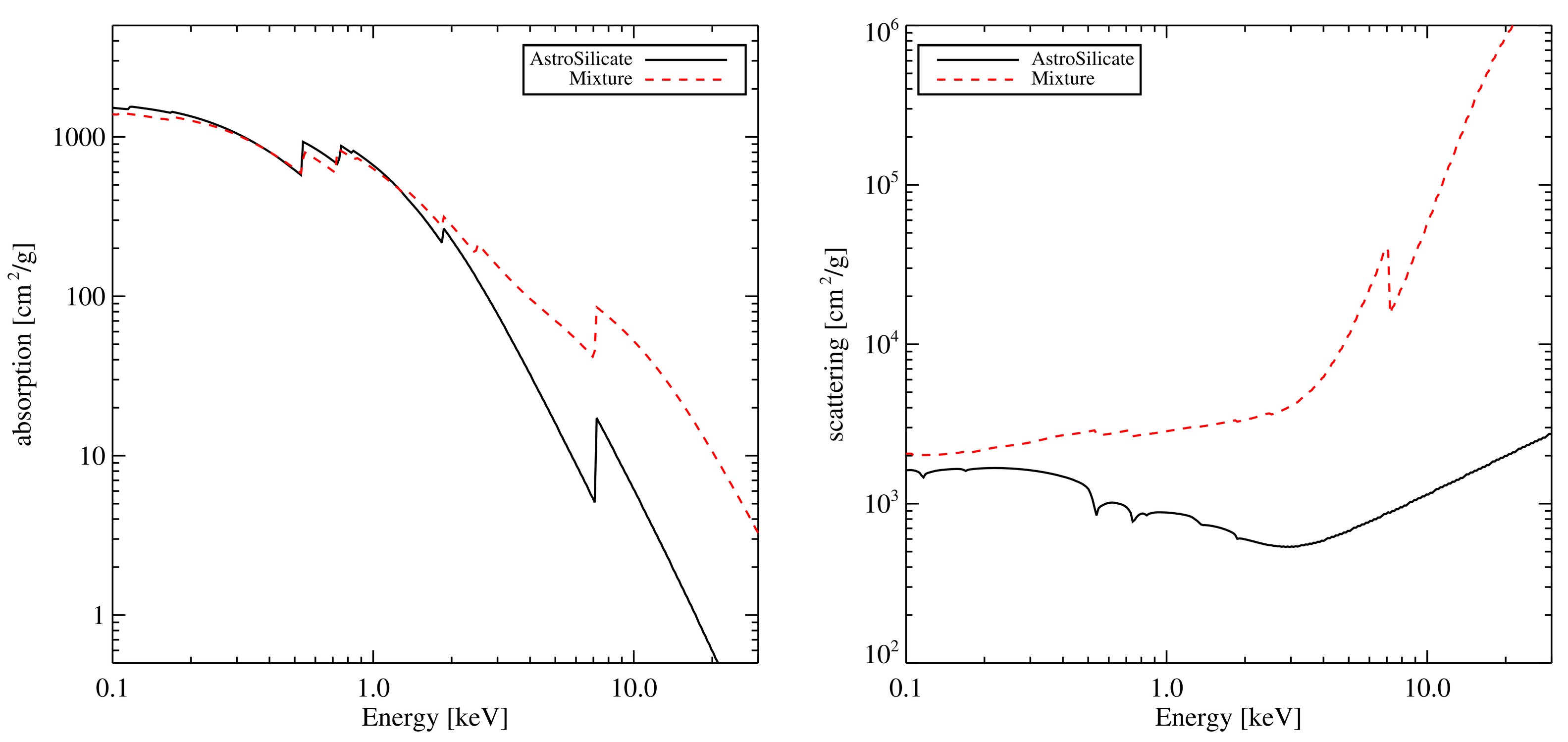

Fig. 1: X-ray dust opacities (*left*: absorption, *right*: scattering): *Astronomical Silicates* compared to a *mixture* of olivine, pyroxene, amorphous carbon and troilite.

- **X-ray Background Radiation Field**
  We consider a possible isotropic X-ray background field in the X-ray RT. An X-ray background field can arise from young embedded star clusters, which produce X-ray fluxes in the range of $10^{-6} \lesssim F_X \lesssim 10^{-4}$ [erg s^{-1} cm^{-2}] (Adams et al., 2012). For the shape of the background spectrum we assume an exponential bremsstrahlung spectrum similar to a stellar X-ray spectrum as the background radiation is produced by young stars.
- **Secondary FUV-field**
  High energy secondary electrons caused by X-ray ionisation can excite H_2 and H, which then produce Lyman-α photons. This secondary FUV-field triggers additional chemical reactions. We duplicate the cosmic ray photon reactions from the UMIST database (Woodall et al., 2007) and calculate the photoreaction rates as outlined in Meijerink & Spaans (2005).

The Disk Model

We present our results for a T-Tauri disk model, which should resemble the properties of a "typical" T-Tauri disk, with the following parameters:

Stellar mass	0.7 $M_\odot$	Fixed disk structure	
$T_{\rm eff}$	4000 K	Inner disk radius	0.07 AU
Stellar lum. L_*	1.0 $L_\odot$	Outer disk radius	400 AU
Disk gas mass	0.01 $M_\odot$	Cosmic ray (CR) ion. rate	1.7×10^{-17} s^{-1}
X-ray lum. L_X	2×10^{30}, 2×10^{31} erg s^{-1}	FUV excess lum. $L_{\rm FUV}/L_*$	0.01

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First Results

In Fig. 2 the X-ray ionisation rate for four different models is shown. For the *absorption only* model no X-ray scattering or background field is included. The *scattering* and *dust* models include scattering by the gas, where for the latter also the dust is considered. The *background* model includes, additionally to the dust model, an X-ray background field as described in the *RT-module* section.

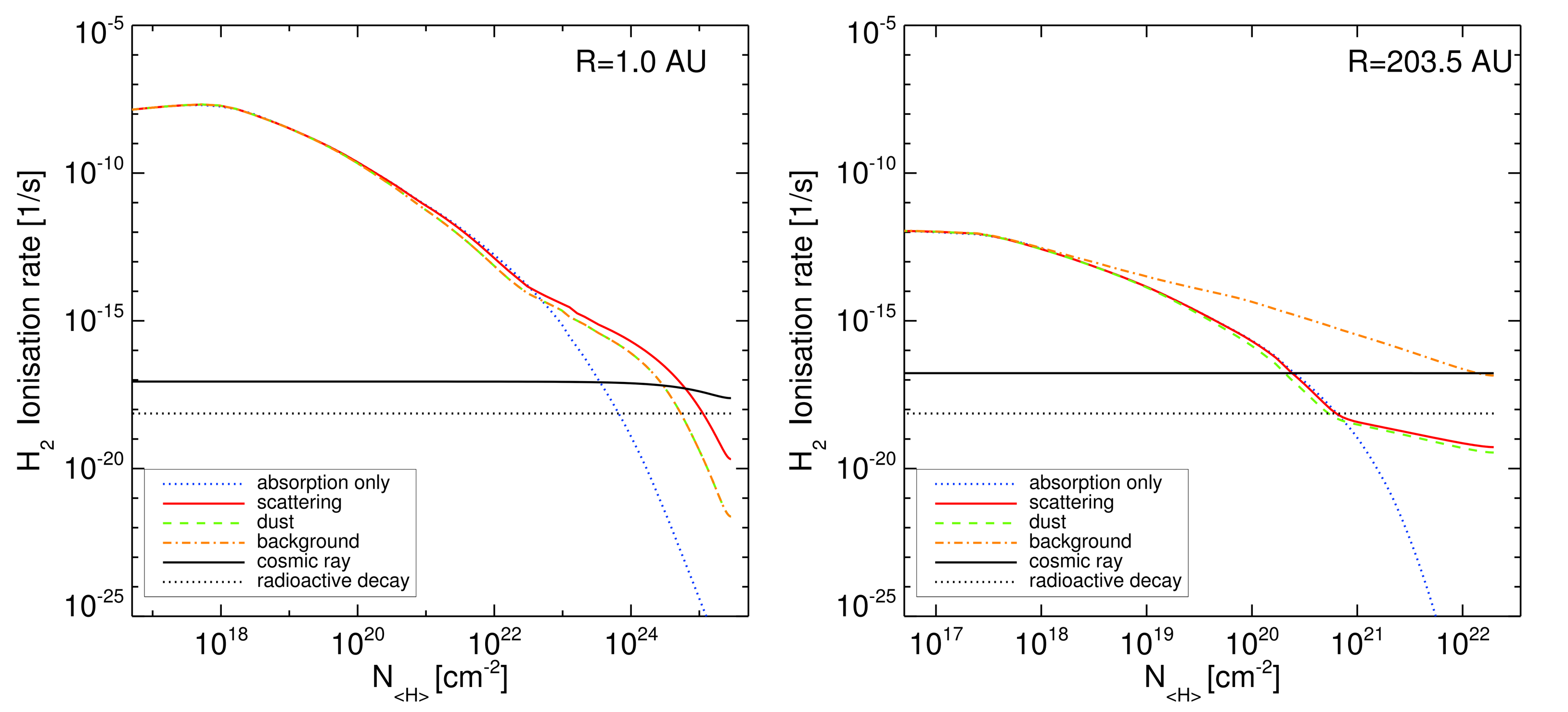

Fig. 2: X-ray ionisation rate for H_2 vs. vertical hydrogen column density for the inner disk (*left panel*) and the outer disk (*right panel*). For comparison also the cosmic ray (CR) and radioactive decay (RD) ionisation rates are given. RD ionisation is not yet included in the models.

For the inner region of the disk ($r \lesssim 10$ AU) **X-ray scattering** somewhat extends the vertical layer where X-ray ionisation is dominant over CR or RD ionisation. For the outer disk region X-ray scattering is not efficient enough (see also Fig. 3). Adding **X-ray dust opacities** does not significantly change the picture. For a dust mixture (see section *RT-module*) instead of *Astronomical Silicate* the scattering due to dust becomes more important but only for a small region close to the inner border of the disk ($r \lesssim 0.5$ AU). For higher X-ray luminosities scattering becomes more important (the affected region is extended) but in general the impact of scattering on the chemistry and line fluxes remains limited.
The **X-ray background radiation field** can be the dominant source for the X-ray ionisation rate in the outer region of the disk ($r \gtrsim 50$ AU), which is roughly in agreement with Adams et al. (2012). As seen in Fig. 2 the X-ray ionisation rate is then stronger than the CR or RD ionisation rates. The X-ray background field can therefore drive additional ion-chemistry and as a result ionized molecules like N_2H^+ (see Fig. 3) or HCO^+ become more abundant. Also the abundance of ionized atoms like C^+, O^+ and doubly ionized species like Fe^{++} or N^{++} is enhanced in this region.

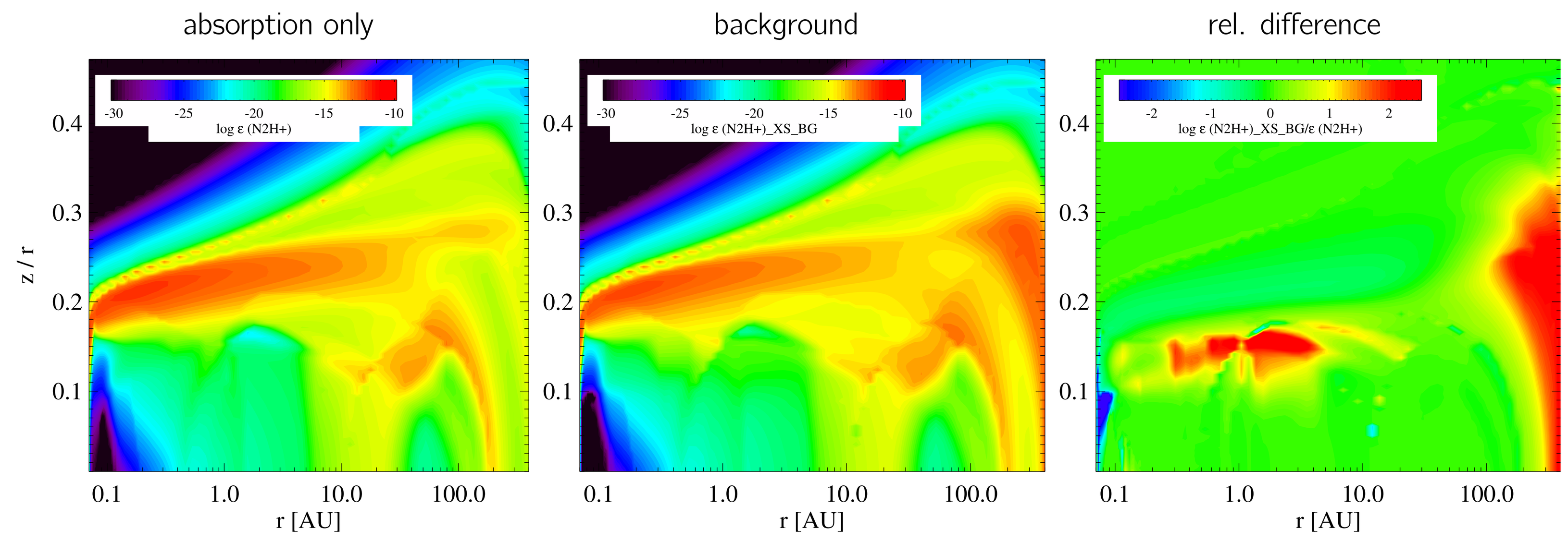

Fig. 3: Relative abundance ϵ of N_2H^+ to H for a model without X-ray scattering (*left panel*) and a model with X-ray scattering and a rather strong background field (*middle panel*). The *right panel* shows the differences of the two models ($\log(\epsilon_{backgr.}/\epsilon_{no\,scat})$, note the different color scale). The x-axis shows the radial distance to the star (*log scale*) and the y-axis the height of the disk scaled by the radius (z/r). Scattering only affects a small region in the inner disk. The background field can drive additional ion-chemistry in the outer parts of the disk which enhances the abundance of N_2H^+ by more than two orders of magnitude.

The **secondary FUV-field** caused by X-rays does not have any significant impact for the models presented here, because CR ionisation remains dominant in the midplane of the disk.
The most affected **spectral lines** in our models are sub-mm lines like N_2H^+ 3 − 2, HCO^+ 3 − 2 and HCO^+ 4 − 3 which are observed in protoplanetary disks. The X-ray background field can raise these line fluxes by up to a factor of 2.5 to 3.5. Atomic lines are not significantly affected (including NeII 12.81 μm) only the CII 157.7 μm line flux becomes stronger by about 30%. Scattering does not have a strong impact on the line fluxes (max. change 30%) as it only affects a small region of the disk.

Summary & Outlook

We presented the new X-ray radiative transfer module for ProDiMo which includes X-ray scattering, a treatment for the secondary FUV radiation field and a possible X-ray background field.
First results show that X-ray scattering only affects the inner region of the disk and therefore the impact on the line fluxes is rather low. The secondary X-ray FUV-field is not important for the kind of models we presented here. Only the X-ray background field can have significant impact on the line fluxes of sub-mm lines like N_2H^+ 3 − 2, HCO^+ 3 − 2 and HCO^+ 4 − 3 (up to a factor of 3.5). We conclude that a X-ray background field might be to some extent a reason for the observed variations in these sub-mm lines for T-Tauri disks (e.g. Öberg et al., 2011).
For the future we plan to include ionisation due to radioactive decay and want to consider possible lower cosmic-ray ionisation rates (Cleeves et al., 2013) as these ionisation sources "compete" with X-ray ionisation. The next steps will than be to fit various disk observations which is the main goal of the **DIANA** (DIsc ANAlysis) project. This will give us deeper insight into the importance and role of X-rays in protoplanetary disks.