The chemistry and dynamics in the region affected by shock and ionization fronts around a young stellar object

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1. Goal of the presentation

We present first results of a self-consistent dynamical and chemical modeling of the shock and ionization front propagation into molecular gas, surrounding a young massive star. The main idea is to describe consistently the development of the structure *"ionization / dissociation / shock / evaporation fronts / cold undisturbed region"* and to evaluate specific details of the evaporation front appearance for the most important astrochemical species, like CO, H_2CO, CH_3OH, NH_3, CS etc. We begin with classical HII regions, but we are very interested in modeling of hcHII and ucHII regions as well. The model can also be used for studies of hot cores around intermediate mass stars.

2. Model

Main ingredients:

Dynamics: publicly available code ZEUS-2D (1D, spherical symmetry)
Chemistry: rate-equation method for gas and solid phases

Initial setup:

1) Star: T_{eff} and surface gravity define specrtum (Kurucz`s models) of a star. We work with massive stars mainly.

2) Gas Environment: Size (from about 0.5 pc to several pc) and number density (from 10^3 to 10^6 cm^{-3}, radius dependent distribution) are specified

3) Chemical composition: Relative abundances for initial HI and H_2 regions (initial abundances for H2 region: x(H2)=0.5, x(CO:d)=$1.8\cdot10^{-4}$, for HI region: x(H)=1, x(C)=x(O)= $1.8\cdot10^{-4}$)

How we calculate chemistry:

1) Photochemistry:
H + ph ⟶ H^+ + e^- + heat
H2 + ph ⟶ H + H + heat
CO + ph ⟶ C + O + heat
C + ph ⟶ C^+ + e^- + heat
etc.
Reaction rates are integrated over stellar spectrum.

2) Interaction with dust:
a) H2 formation
b) Accretion and desorption (photo, thermal and induced by cosmic rays)

3) All other two-body reactions:
rates from the UMIST database

How we calculate dust temperature:

1) Radiative balance

$$\int Q_\nu^{abs}(a)\cdot J_\nu\,d\nu = \int Q_\nu^{abs}(a)\cdot B_\nu(T_d)\,d\nu$$

2) Interaction with gas particles by collisions

How we calculate gas temperature:

We added several heating and cooling mechanisms to the ZEUS code:
1) *Chemistry-dependent contribution* (like H⟷H^+, H2⟷H + H, C⟶C^+ etc.)
2) $Lyman_\alpha$ emission, free-free electron transitions, FUV pumping of H_2, fine-structure and forbidden transitions of OI, OII and CII, vibrational and rotational transitions of CO, H_2O and H_2

How the code works:

We calculate several sets of equations step by step:

Chemistry: UMIST reactions and photoreactions (without H⟷H^+, H_2⟶H + H reactions, they influence the thermal balance significantly)

↓

Chemistry (H⟷H^+, H_2⟶H + H) + *heating and cooling*

↓

Dynamics (ZEUS-based part)

3. First Results

Results of the test calculations with uniform density distribution ($n(H+H2)_{init}$ = $3\cdot10^4$ cm^{-3}) are presented here. List of chemical reactions considered so far is presented in Table 1. Typical physical and chemical structure in the vicinity of a young massive star with T_{eff} = 30000K is shown in Fig. 1. Physical values have arbitrary scales. Radial profiles of gas temperature and density can be divided into several regions as described in Fig. 1. Fronts of ionization, dissociation and evaporation of species are also shown, values of abundances are scaled.

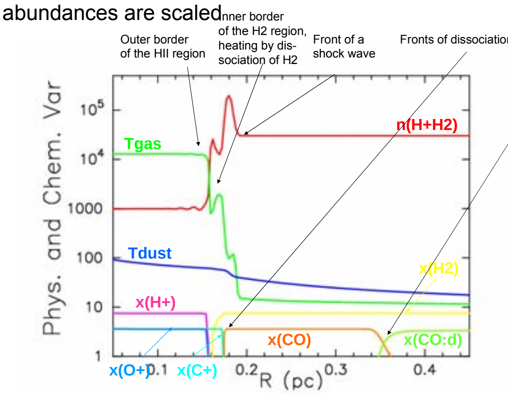

Fig. 1: Typical physical and chemical structure of a gas-dust envelope In the vicinity of a young massive star with T_{eff} = 30 000K at time = $3\cdot10^4$ years

If we do not include desorption by cosmic rays, we obtain a structure similar to a developed HII region directly surrounded by a cold region without gas phase CO as is shown in Fig. 2 (left panels). Such a structure is not consis-tent with observational results (see, for example, a poster "Triggered star formation in S235" of Kirsanova et al.)

H + ph ⟷ H^+ + e^-
H_2 + ph ⟶ H + H
H:d + H:d ⟶ H_2
CO + ph ⟷ C + O
C + ph ⟷ C^+ + e^-
H^+ + O ⟷ H + O^+
H:d ⟷ H
CO:d ⟷ CO
C:d ⟷ C
O:d ⟷ O

Tab. 1. Chemical reactions included in the model

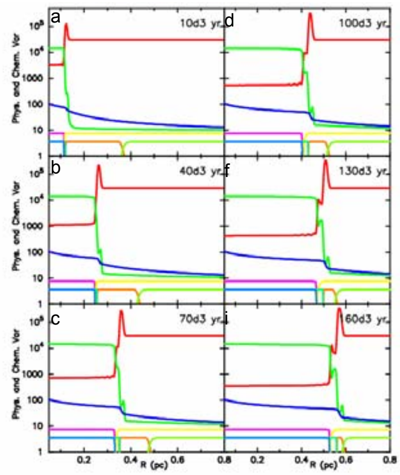

Fig. 2: Evolution of the structure for a star with T_{eff} = 30 000K for several time moments

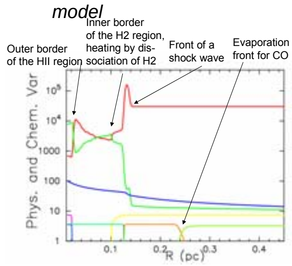

Fig. 3: Physical and chemical structure of a gas-dust envelope around a young massive star with Teff = 20 000K at time = 4·104 years

If we consider a star with Teff=20000K, which corresponds to a less massive star (~ 8 $M_\odot$) we have a similar structure, but the size of the HII region is much larger than in the case of T_{eff}=30000K (compare Fig.3 and Fig. 2b). This is reflected on radial profiles of temperature and density.

Influence of an intermediate-mass star (T_{eff}=10000K, M = 3 $M_\odot$) on its environment is shown in Fig. 4. There is no HII region, but the outward propagation of gas is visible because of heating by formation of C^+. Abundance of gas phase CO is enhanced in cold region because we included cosmic ray desorption in this model.

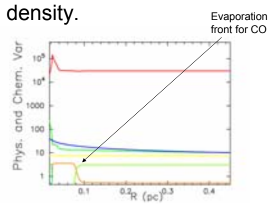

Fig. 4: Physical and chemical structure of a gas-dust envelope around a young massive star with Teff = 10 000K at time = $7\cdot10^4$ years

4. Plans for the near future

We are going to consider the development of such a physical and chemical structure with various types of radial density distribution (like $n \sim r^{-\alpha}$) and more diverse chemical composition (add H_2CO, CH_3OH and related species first of all).

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