Chemical evolution in C-type shock waves

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The shock waves of C-type ('continuous') and J-type ('jump')

The sound speed in the neutral component of the gas:

$$v_{\rm s} = \left(\frac{5kT}{3\mu_n}\right)^{1/2}$$

Ion magnetosonic speed:

$$v_{\rm ims} = \left[\frac{B^2/(4\pi) + 5/3(n_i + n_e)kT}{\rho_i + \rho_e + B^2/(4\pi c^2)}\right]^{1/2}$$

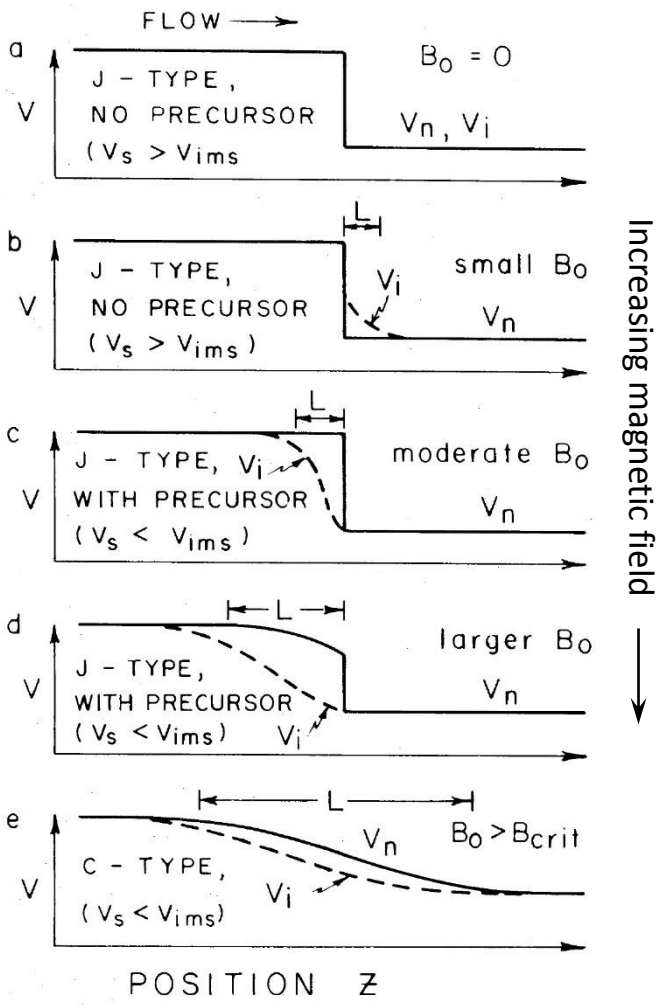
If the speed of the gas flow satisfies the condition:

$$v_{\rm s} < u < v_{\rm ims}$$

– the C-type shock forms. The C-type shocks are non-dissociative – molecules survive the passage of the shock wave.

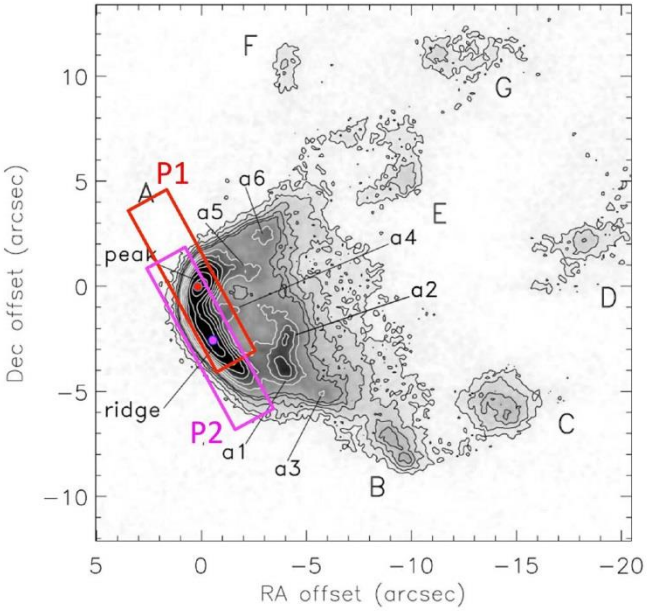
If the gas temperature in the shock is high enough for the H_2 dissociation (that is the main cooling agent) – the temperature and ionization fraction of the gas increase, the shock wave becomes a J-type. Maximal (critical) speeds of C-type shocks lie in the range 40-60 km/s (Draine 1993; Le Bourlot et al. 2002).

The effect of magnetic field on the structure of the shock wave (Draine,1980):

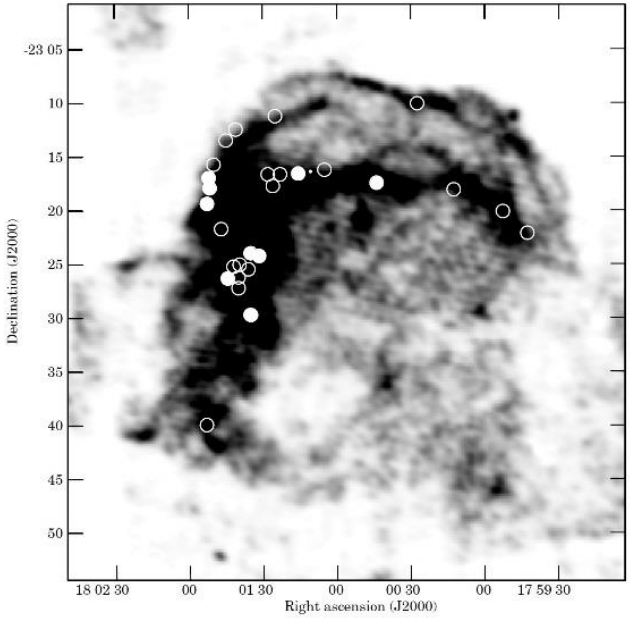


C-type shocks in astronomical objects:

1. The interaction between protostellar outflows and ambient interstellar medium. In the figure – HH7, a bow shock that is driven by a jet from the young stellar object (YSO) SVS 13 (Neufeld et al. 2019).



2. The interaction between a supernova remnant and a dark molecular cloud. The supernova remnant W28 is shown in the figure, the OH masers are designated by white circles (Pihlstrom et al., 2014).



Other sources of shocks in the interstellar medium:

3. Cloud–cloud collisions (Requena-Torres et al., 2006)
4. The dissipation of turbulence (Godard et al. 2014)

Shock modelling

Numerical models of shock waves usually consider in detail either the gas dynamics, but reduced chemical network is used:

Flower and Pineau des Forêts (2015);

or vice versa – the parametric model of the steady state profile of the shock is used to study in detail the chemical evolution of the gas:

Holdship et al. (2017);

Burkhardt et al. (2019).

The advantage of a magnetohydrodynamic model over the parametric one is that a large number of physical parameters (e.g., cosmic ray ionization rate, intensity of interstellar background radiation field, dust properties, and etc.) may be varied.

The physics included in the model

Here, we present a magnetohydrodynamic (MHD) model of C-type shock coupled to a full gas–grain chemical network. The main physical processes are included:

- MHD equations are solved
- molecular excitation (H_2, CO, H_2O, OI, CI, CII)
- full gas–grain chemical network (gas-phase chemistry UDfA, grain surface chemistry network from NAUTILUS)
- sputtering of icy mantles of dust grains
- collisional dissociation of molecules at high gas temperature

The details of the simulations are published in

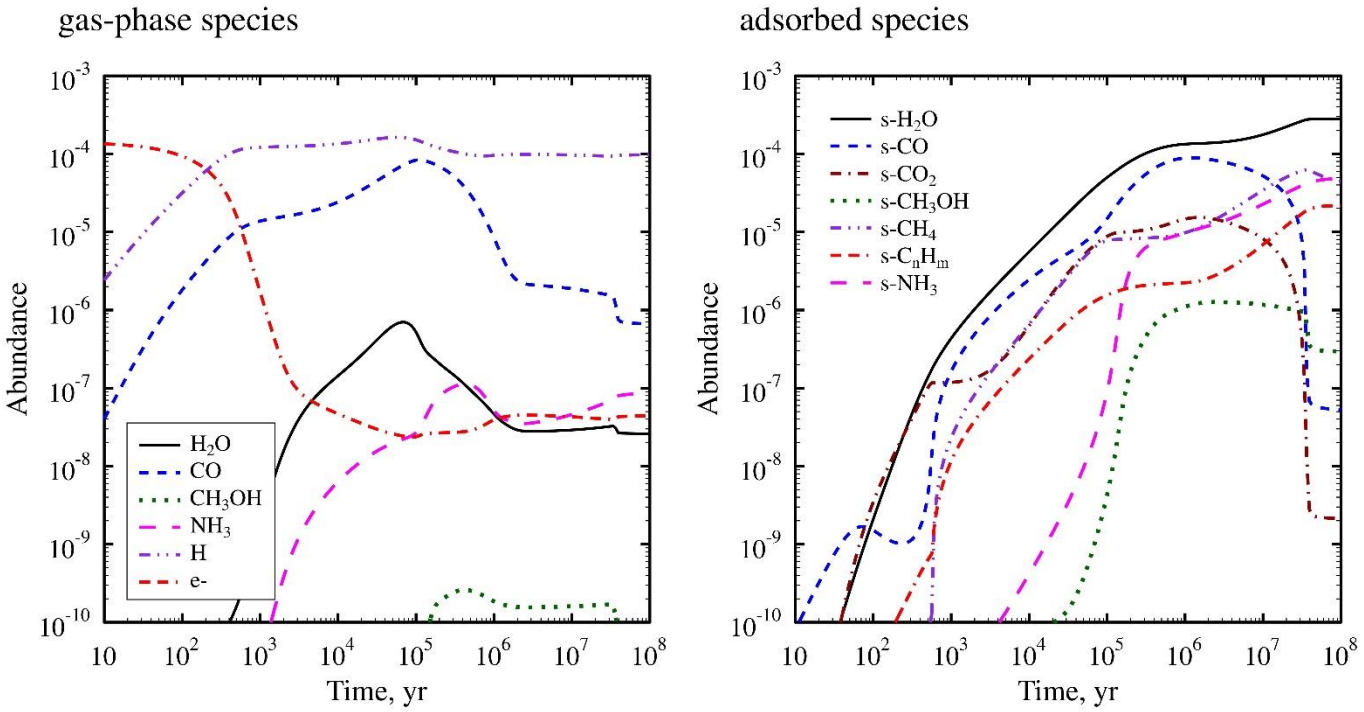
Nesterenok A.V. Astrophysics and Space Science 2018, **363**,151.

Results of chemical evolution of a dark molecular cloud

The objectives of the modelling of the chemical evolution of a static dark cloud are:

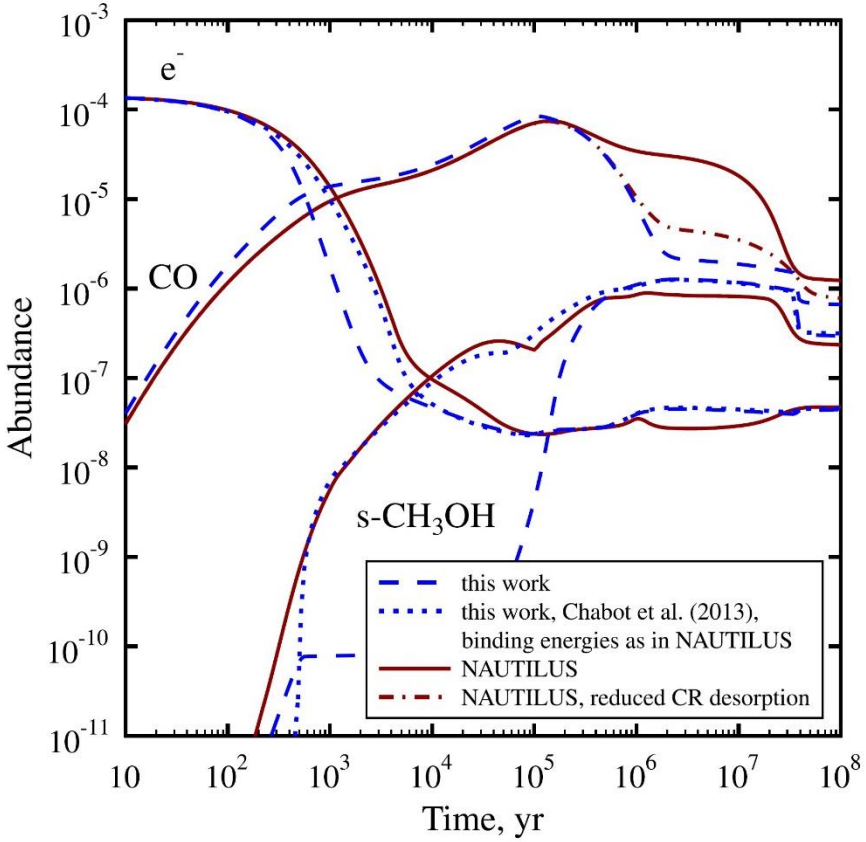
(i) verification of our chemical model;

(ii) evaluation of the chemical composition of the gas before the shock wave propagates through it.



The results are ‘standard’, see discussion by Nesterenok (2018). The chemical evolution of dark molecular clouds was studied by many workers.

Comparison with NAUTILUS



Comparison of our simulation results with NAUTILUS results. The results of simulations are also shown with updated chemical network according to Chabot et al. (2013) and using the data on specimen binding energies as in NAUTILUS model. The results of NAUTILUS model with direct cosmic ray desorption reduced by an order of magnitude are shown.

The number of chemical species, for which the abundance ratio:
< 2 – about 100
> 2, but < 10 – about 150

The differences between our model and NAUTILUS:

- NAUTILUS uses the astrochemical database KIDA. While our code uses UMIST Database for Astrochemistry (UDfA).
- The data on binding energies by Penteado et al. (2017) are used here;

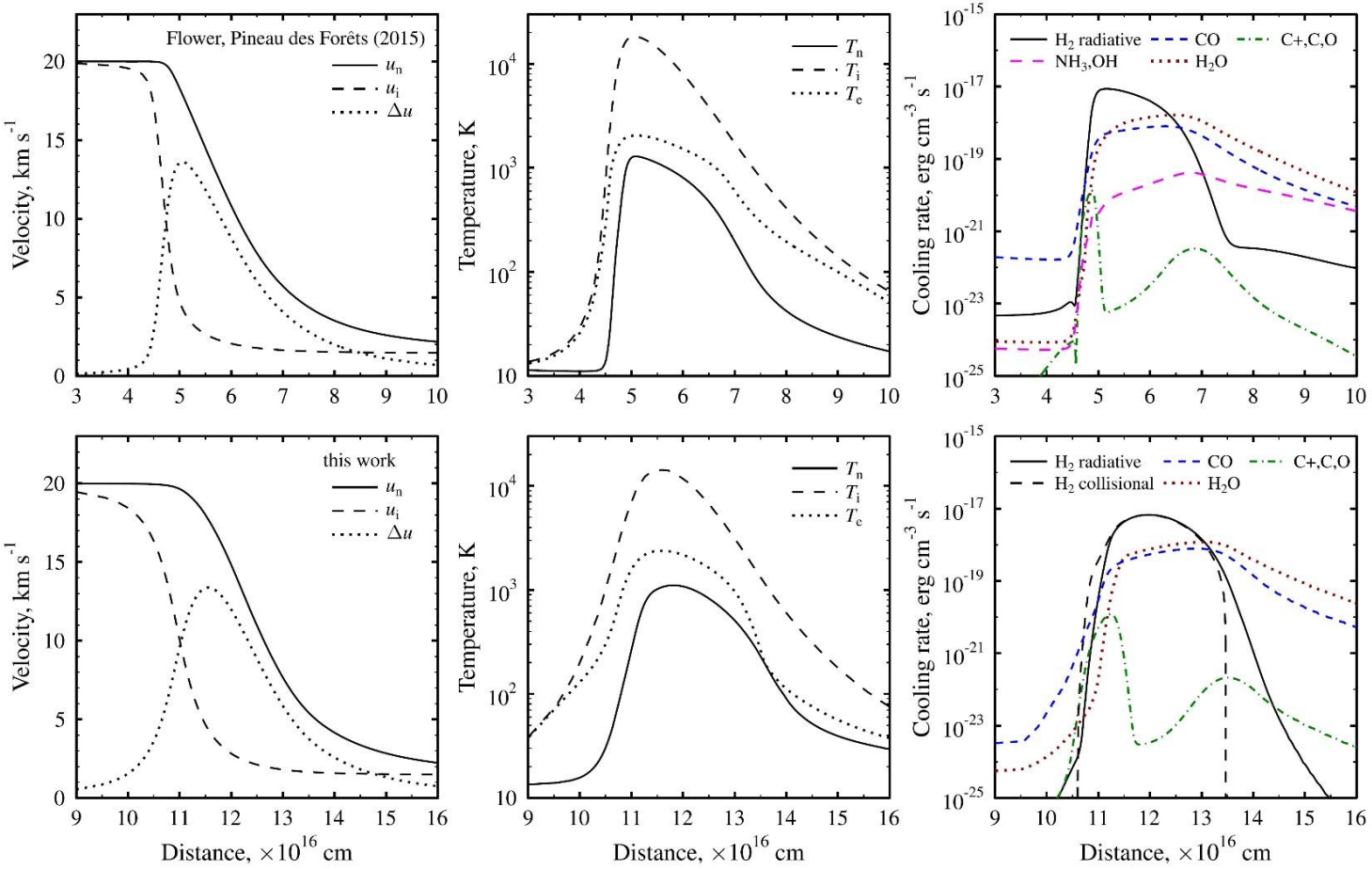
The example,
UDfA:

$$C_n^- + C^+ \rightarrow C_n + C$$

KIDA, Chabot et al. (2013):

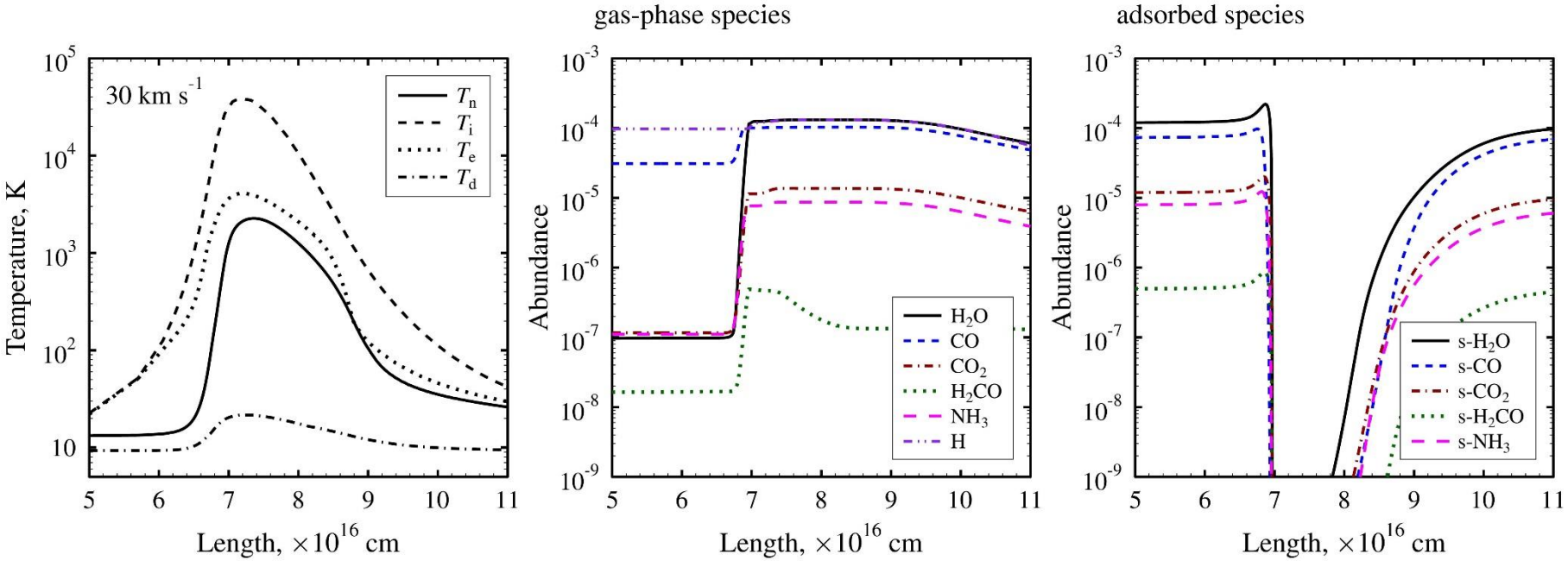
$$C_n^- + C^+ \rightarrow C_k + C_l + C_m$$

Comparison with the shock model by Flower and Pineau des Forets (2015) (‘Paris–Durham’ model)



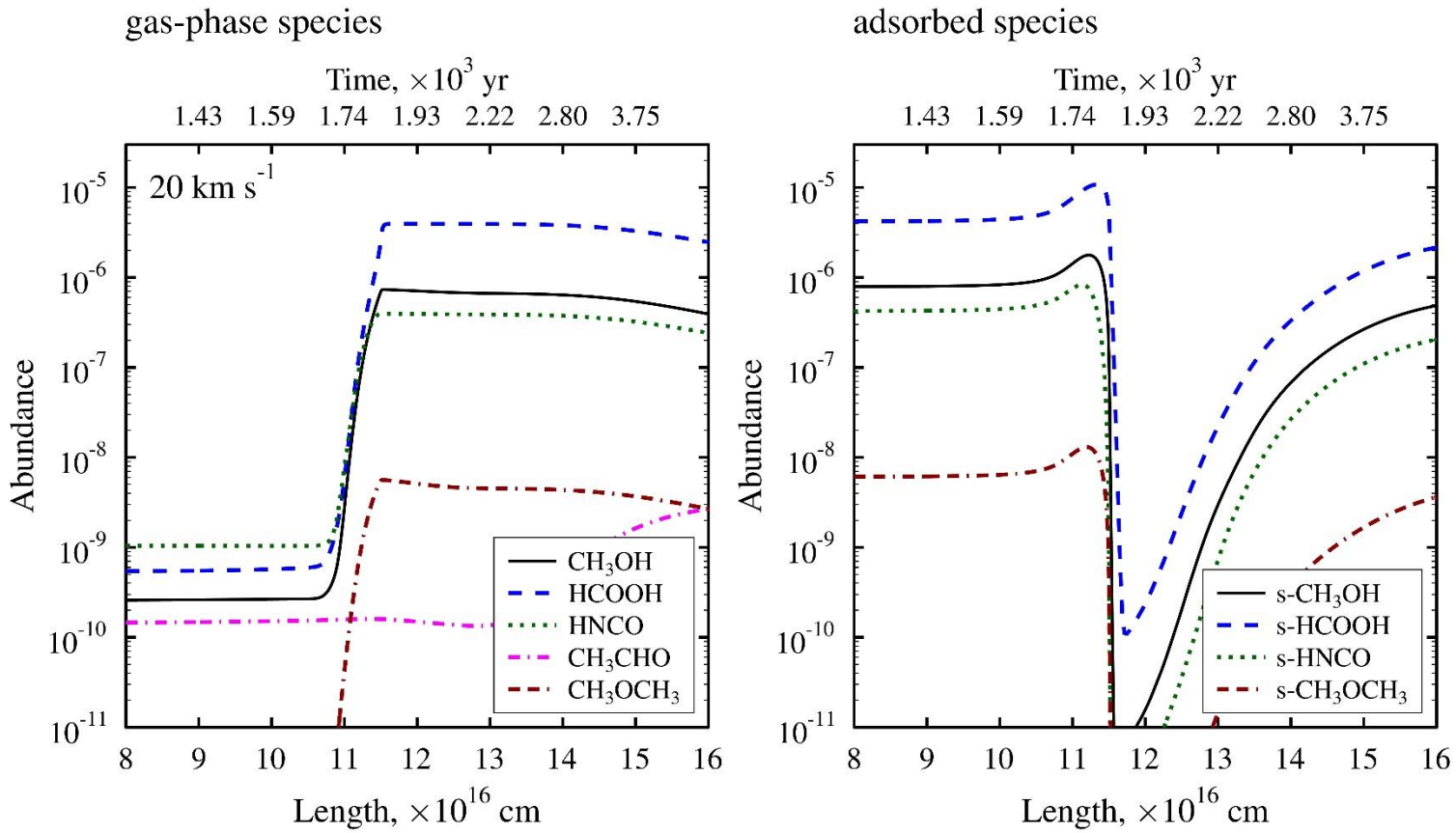
The general behaviour of physical parameters is similar in our model and that by Flower and Pineau des Forêts (2015). The shock model by Flower and Pineau des Forêts (2015) does not consider grain surface chemistry and includes simpler gas-phase chemical network than our model – the effect of expanded chemistry on shock structure is minimal.

Chemical evolution of the gas in C-type shock – simple species



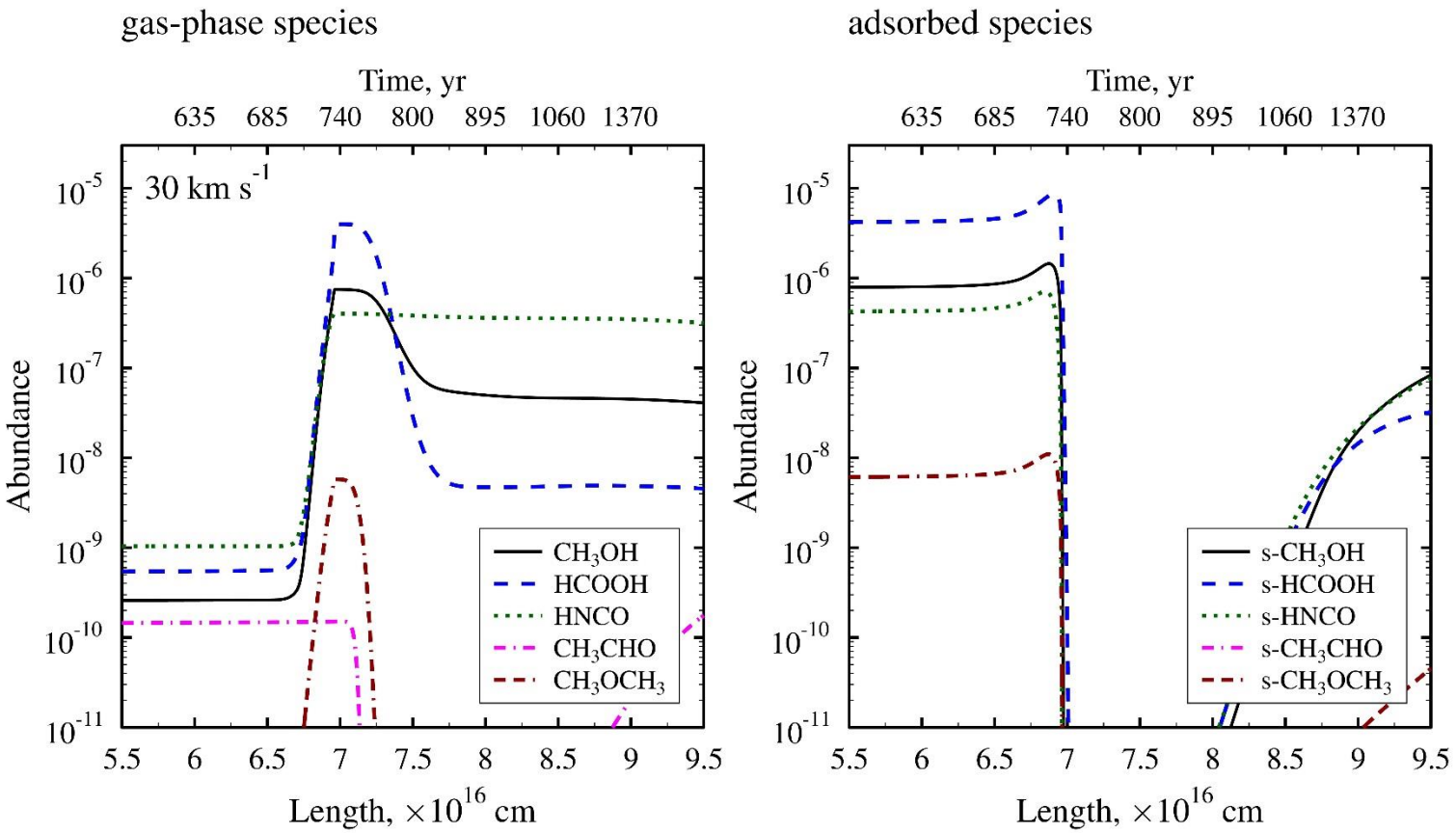
The simulation results on abundances of simple species are in agreement with the findings by other workers, see e.g., Bergin et al. (1998), Charnley and Kaufman (2000), Viti et al. (2011), Flower and Pineau des Forêts (2012).

Complex organic molecules – shock speed 20 km/s



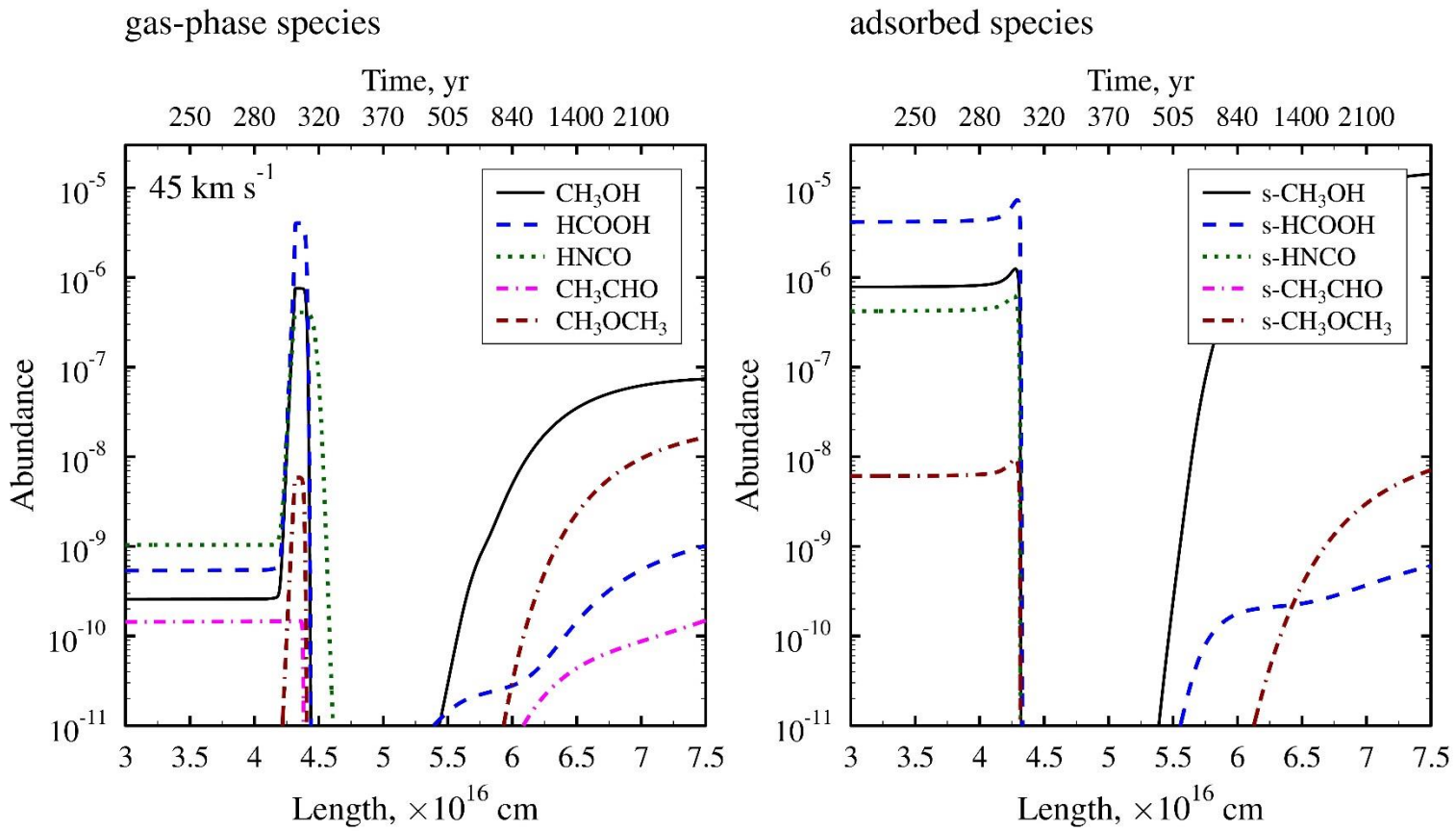
The abundance of complex organic molecules in the gas phase at the shock front increases by many orders of magnitude due sputtering of icy mantles of dust grains. Molecules survive the passage of the shock, and the abundances of species are relatively high in the postshock region.

Complex organic molecules – shock speed 30 km/s



The sputtering of grain mantles takes place in the region close to the temperature peaks of neutral gas and ions. At high shock speeds, molecules are destroyed in the hot shocked gas via reactions with H atoms and collisional dissociation reactions. The survival time of complex molecules in the hot gas is low – of the order of dozens of years. This contradicts the conclusions by Palau et al. (2017) who used the parametric model of C-type shock.

Complex organic molecules – shock speed 45 km/s



At high shock speeds, there is high abundance of atomic hydrogen in the gas produced in collisional dissociation reactions. It triggers formation of complex molecules on the grain surface such as CH_3OH. COMs are effectively produced in the gas phase in the postshock region. The main parent species in the gas-phase synthesis of COMs are H_2CO, CH_3OH, C_2H_4 and radicals CH_3, CH_3O, C_2H_5.

Conclusions

1. At high shock speeds, molecules ejected from icy mantles are destroyed in the hot gas, and their survival time is low. These results imply that strict constraints must be put on the physical parameters for the shock regions where large astronomical molecules are observed − shock velocity and gas density must be low enough to allow molecules survive in the hot shocked gas.
2. After a passage of high-speed C-type shock, a gas layer of high abundance of atomic hydrogen appears in the cooling postshock gas, that triggers formation of large organic species.
3. Gas-phase methanol is re-formed via reactive desorption mechanism. The efficiency of reactive desorption is a key parameter that determines the gas-phase abundance of methanol and other complex species that are produced via it.
4. These results are important for interpretation of observations of the molecular emission in protostellar outflows and supernova remnants.

Thank you for attention