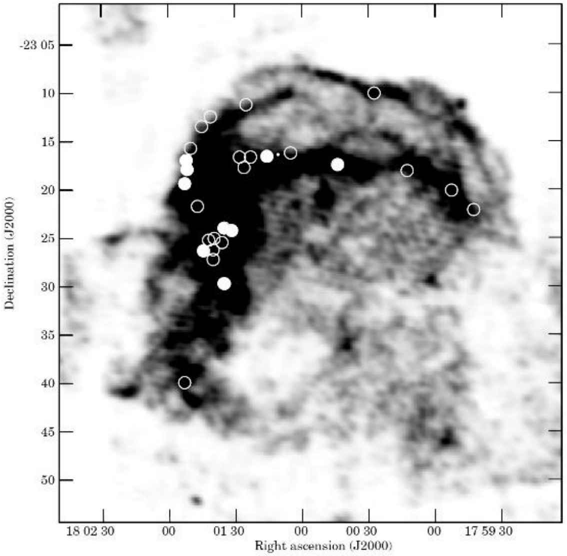
Modelling C-type shocks in interstellar clouds

Aleksandr Nesterenok (Ioffe Institute, St. Petersburg)

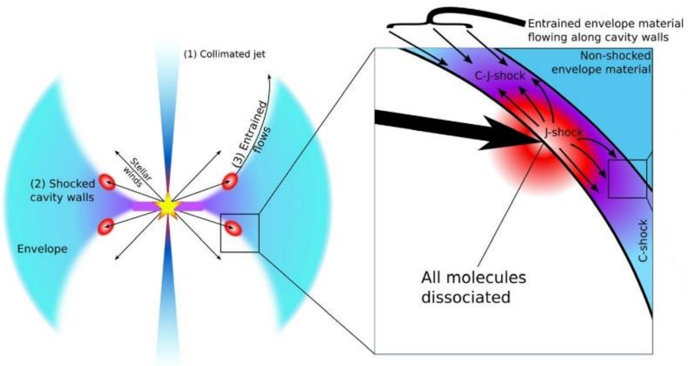
Sources of Interstellar Shocks

1. Supernova remnants



The figure shows supernova remnant W28. Grayscale map in the 327 MHz continuum, regions where OH masers are located are marked with filled circles (Pihlstrom et al., 2014). OH masers mark the interaction of the supernova shock with the molecular cloud.

2. Protostars
The gas in fast stellar winds is eventually decelerated when it “runs into” the ISM; the deceleration involves passage of the wind material through a shock front.



(Suutarinen et al., 2014)

3. Collisions of interstellar clouds (Requena-Torres et al., 2006)
4. Expanding HII regions can drive shock waves into surrounding neutral gas.

Shock waves

A shock wave is a pressure-driven disturbance propagating faster than the signal speed for compressive waves, resulting in an irreversible change.

- relativistic shocks, $u \sim c$
- non-relativistic, J-type shocks, $c >> u > 40–60$ km/s
  J means “jump” – the sharp change in fluid properties (density, velocity, pressure) in a shock transition.
- two-fluid MHD C-type shocks, $u < 40–60$ km/s
  C means “continuous”, the momentum transfer and dissipation take place as the result of ion–neutral streaming in an extended region of interstellar gas.

Shock waves process the gas:

- change density, velocity and temperature
- affect ionization state, destroy dust grains, drive chemistry
- particle acceleration
- shocked gas radiates

Two-Fluid MHD shocks in low fractional ionization gas

The gas can be thought of as two distinct fluids: a neutral fluid consisting of atoms and molecules, and a plasma, consisting of the ions, electrons, and magnetic field.

Sound speed in neutral gas is:

$$v_\mathrm{s} = \left(\frac{5kT}{3\mu_n}\right)^{1/2} \simeq 3\,\mathrm{km\,s^{-1}} \left(\frac{T}{1000}\right)^{1/2}$$

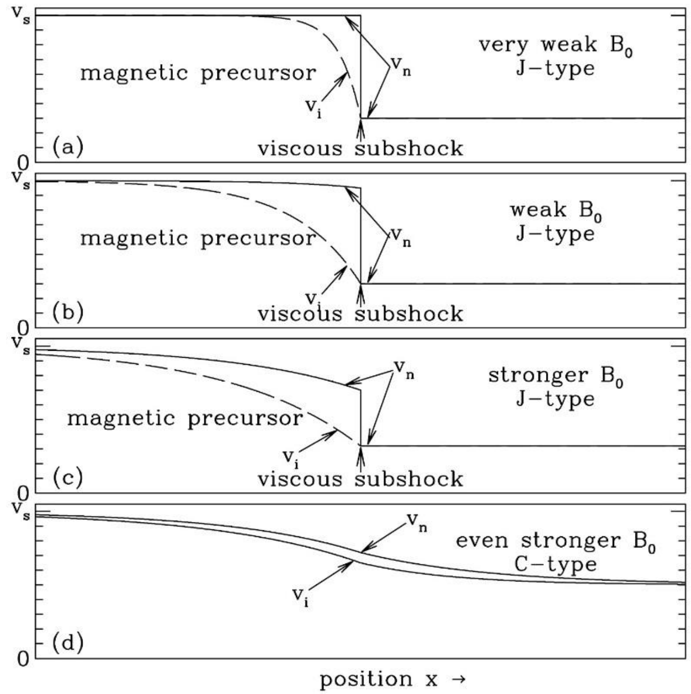
Magnetosonic speed for compressive waves in the plasma is:

$$V_\mathrm{ims} \approx \frac{B_0}{\sqrt{4\pi\rho_i}} \approx 112\,\mathrm{km\,s^{-1}} \left(\frac{B_0}{5\,\mu\mathrm{G}}\right) \left(\frac{10^2\,\mathrm{cm}^{-3}}{n_\mathrm{H}} \frac{10^{-4}}{x_i}\right)^{1/2}$$

If the shock speed $v_s < u_s < V_{ims}$, then compressive waves in the plasma can propagate upstream ahead of the shock, producing compression in the plasma before it arrives at the shock transition – C-type shock forms.

If the gas temperature becomes high enough for H_2 molecule dissociation – the temperature and ionization rise, shock becomes J-type. Limiting velocities for C-type shocks are about 40–60 km/s (Draine, 1993).

The influence of magnetic field strength on shock structure (Draine, 2011):



C-type shock waves in molecular clouds

Example of C-type shock – interaction of old supernova shock with molecular cloud

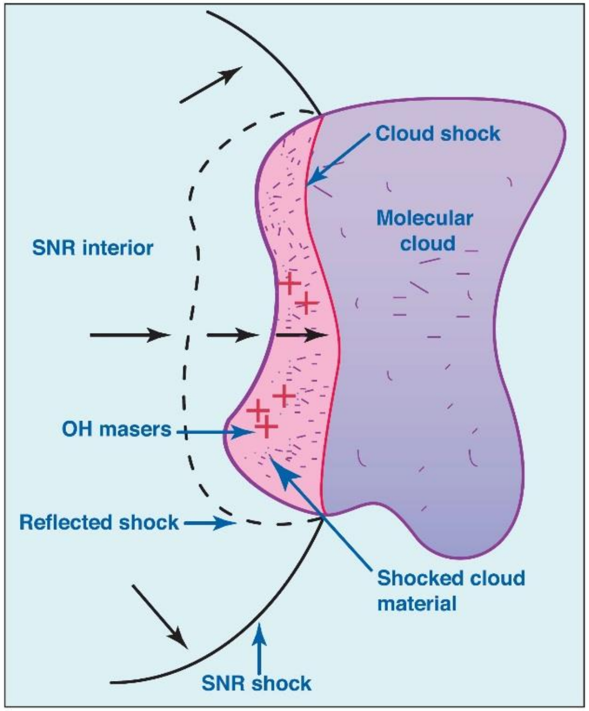


Fig. 1. Schematic of an expanding supernova remnant (SNR) interacting with an adjacent molecular cloud. Black arrows indicate velocity.

Wardle, Science 296, p.2350, 2002

Parameters of cloud cores:

- densities $10^4 – 10^6$ cm^{-3},
- low ionization degree, ~ $10^{-8} – 10^{-7}$,
- magnetic fields B $\sim\sqrt{n[\mathrm{cm}^{-3}]}$ [μG],
- "ambipolar diffusion"
  ions interact with magnetic field, neutrals interact with ions via collisions, charged particles drift through the neutrals;

One of the motivations of this work is to investigate the chemical processing of the gas during the star formation, in particular, formation and destruction of complex molecules, e.g. relevant for the life genesis.

Description of the model. The MHD equations

The equations of conservation of particle number, mass, momentum, energy (Draine et al., 1983):

$$\frac{\mathrm{d}}{\mathrm{dz}}\left(\frac{\rho_{\mathrm{n}}}{\mu_{\mathrm{n}}}u_{\mathrm{n}}\right)=\mathcal{N}_{\mathrm{n}} \qquad \frac{\mathrm{d}}{\mathrm{dz}}\left(\frac{\rho_{\mathrm{i}}}{\mu_{\mathrm{i}}}u_{\mathrm{i}}\right)=\mathcal{N}_{\mathrm{i}}$$

$$\frac{\mathrm{d}}{\mathrm{dz}}\left(\rho_{\mathrm{n}}u_{\mathrm{n}}\right)=\mathcal{S}_{\mathrm{n}} \qquad \frac{\mathrm{d}}{\mathrm{dz}}\left(\rho_{\mathrm{i}}u_{\mathrm{i}}\right)=\mathcal{S}_{\mathrm{i}}$$

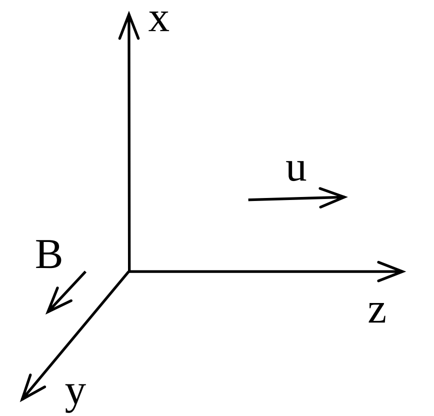
$$\frac{\mathrm{d}}{\mathrm{dz}}\left(\rho_{\mathrm{n}}u_{\mathrm{n}}^2+k_{\mathrm{B}}T_{\mathrm{n}}\frac{\rho_{\mathrm{n}}}{\mu_{\mathrm{n}}}\right)=\mathcal{F}_{\mathrm{n}}$$

$$\frac{\mathrm{d}}{\mathrm{dz}}\left(\rho_{\mathrm{i}}u_{\mathrm{i}}^2+k_{\mathrm{B}}T_{\mathrm{i}}\frac{\rho_{\mathrm{i}}}{\mu_{\mathrm{i}}}+k_{\mathrm{B}}T_{\mathrm{e}}n_{\mathrm{e}}+\frac{B_0^2u_{\mathrm{s}}^2}{8\pi u_{\mathrm{i}}^2}\right)=-\mathcal{F}_{\mathrm{n}}$$

$$\frac{\mathrm{d}}{\mathrm{dz}}\left[\frac{1}{2}\rho_{\mathrm{n}}u_{\mathrm{n}}^3+\frac{5}{2}k_{\mathrm{B}}T_{\mathrm{n}}\frac{\rho_{\mathrm{n}}}{\mu_{\mathrm{n}}}u_{\mathrm{n}}\right]=\mathcal{G}_{\mathrm{n}}+\mathcal{F}_{\mathrm{n}}u_{\mathrm{n}}-\frac{1}{2}\mathcal{S}_{\mathrm{n}}u_{\mathrm{n}}^2$$

$$\frac{\mathrm{d}}{\mathrm{dz}}\left(\frac{1}{2}\rho_{\mathrm{i}}u_{\mathrm{i}}^3+\frac{5}{2}k_{\mathrm{B}}T_{\mathrm{i}}\frac{\rho_{\mathrm{i}}}{\mu_{\mathrm{i}}}u_{\mathrm{i}}+\frac{5}{2}k_{\mathrm{B}}T_{\mathrm{e}}n_{\mathrm{e}}u_{\mathrm{i}}+\frac{B_0^2u_{\mathrm{s}}^2}{4\pi u_{\mathrm{i}}}\right)=\mathcal{G}_{\mathrm{i}}+\mathcal{G}_{\mathrm{e}}-\mathcal{F}_{\mathrm{n}}u_{\mathrm{i}}-\frac{1}{2}\mathcal{S}_{\mathrm{i}}u_{\mathrm{i}}^2$$

$$\frac{\mathrm{d}}{\mathrm{dz}}\left(\frac{3}{2}k_{\mathrm{B}}T_{\mathrm{i}}\frac{\rho_{\mathrm{i}}}{\mu_{\mathrm{i}}}u_{\mathrm{i}}-\frac{3}{2}k_{\mathrm{B}}T_{\mathrm{e}}n_{\mathrm{e}}u_{\mathrm{i}}\right)+\left(k_{\mathrm{B}}T_{\mathrm{i}}\frac{\rho_{\mathrm{i}}}{\mu_{\mathrm{i}}}-k_{\mathrm{B}}T_{\mathrm{e}}n_{\mathrm{e}}\right)\frac{\mathrm{du_i}}{\mathrm{dz}}=\mathcal{G}_{\mathrm{i}}-\mathcal{G}_{\mathrm{e}}$$



It is assumed that magnetic field lines are frozen into the plasma

$N_{\mathrm{i}}, N_{\mathrm{n}}$ – numbers of ions and neutral particles created per unit volume and time;

$S_{\mathrm{i}}, S_{\mathrm{n}}$ – mass source terms describing how much neutral mass is converted into ion-electron mass and conversely;

F_{n} – momentum transferred from the ion-electron fluid to the neutral fluid;

$G_{\mathrm{i}}, G_{e}, G_{\mathrm{n}}$ – energy source terms for the ion, electron and neutral fluid;

Astrochemistry

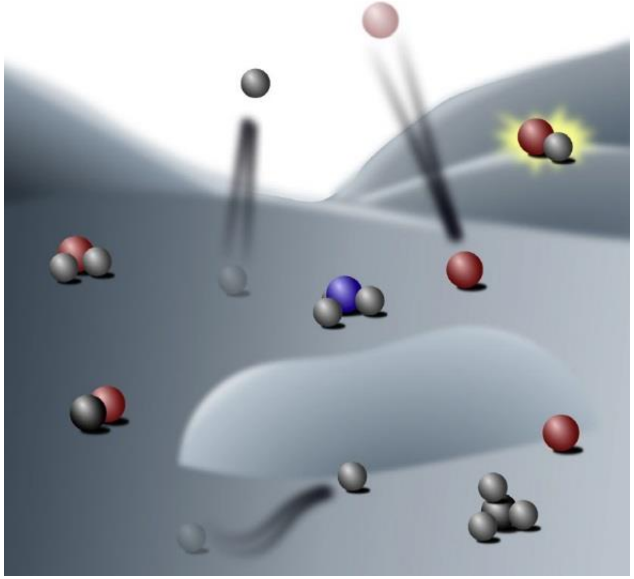
1. Gas-phase chemistry

The data on chemical reactions were taken from UMIST Database for Astrochemistry, the network was supplemented by collisional dissociation reactions. We take into account 426 atoms and molecules (containing H, He, C, N, O, Si, S, Fe, Na, Mg, Cl), about 6000 gas-phase chemical reactions.

2. Gas–grain interactions (adsorption and desorption)

3. Chemistry on dust grains

Bimolecular grain surface reactions were taken from code NAUTILUS (Ruaud et al., 2016), the most of network are reactions that include atoms and light molecules H, H_2, C, O, OH, CH, NH.



Cuppen et al., Space Sci. Rev., 2017

The new feature of these simulations – MHD model is coupled to the full gas-phase and grain surface chemistries. In previous studies of shocks either the accurate gas dynamics is considered, but reduced chemical network is used, or vice versa.

Calculation of level populations of atoms and molecules

The population densities of atoms CI, CII, OI, and molecules H_2, H_2O, CO are considered.

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(\chi_{\mathrm{jm}} u_\alpha\right) = \sum_{l=1,\, l\neq m}^{M} \left(R_{\mathrm{lm}} + C_{\mathrm{lm}}\right)\chi_{\mathrm{jl}} -$$

$$-\chi_{\mathrm{jm}} \sum_{l=1,\, l\neq m}^{M} \left(R_{\mathrm{ml}} + C_{\mathrm{ml}}\right) + \bar{\chi}_{\mathrm{jm}} \mathcal{N}_{\mathrm{j}}, \quad m = 1, ..., M,$$

The Sobolev approximation is used. The radiation intensity averaged over the direction and over
the line profile:

$$J_{\mathrm{lm}}(z) = S_{\mathrm{L}}(z)\left[1 - 2\mathscr{P}\left(\gamma_{\mathrm{L}}, \gamma_{\mathrm{C}}\right)\right]$$

$$\frac{1}{\gamma_{\mathrm{L}}} = k_{\mathrm{L}} \Delta z_{\mathrm{D}}, \quad \frac{1}{\gamma_{\mathrm{C}}} = k_{\mathrm{C}} \Delta z_{\mathrm{D}}$$

The cooling of the gas due to emission in molecular and atomic lines:

$$\mathcal{G}_{\mathrm{j,rad}} = \sum_{\mathrm{l>m}} h\nu_{\mathrm{lm}} \left(C_{\mathrm{lm}}\chi_{\mathrm{jl}} - C_{\mathrm{ml}}\chi_{\mathrm{jm}}\right)$$

Table 4. Data on collisional rate coefficients

Specimen	Collisional partner	Reference
O I	H_2	Jaquet et al. (1992)
		Glover & Jappsen (2007)
	He	Monteiro & Flower (1987)
	H	Krems, Jamieson & Dalgarno (2006)
		Abrahamsson, Krems & Dalgarno (2007)
	e^-	Berrington & Burke (1981)
		Pequignot (1990)
		Bell, Berrington & Thomas (1998)
C I	H_2	Schroder et al. (1991)
	He	Staemmler & Flower (1991)
	H	Abrahamsson, Krems & Dalgarno (2007)
	e^-	Johnson, Burke & Kingston (1987)
C II	H_2	Flower & Launay (1977)
		Draine (2011)
	H	Barinovs et al. (2005)
	e^-	Tayal (2008)
		Draine (2011)
H_2	H_2	Flower & Roueff (1998)
		Flower & Roueff (1999)
	He	Flower, Roueff & Zeippen (1998)
	H	Lique (2015)
		Wrathmall, Gusdorf & Flower (2007)
		Martin & Mandy (1995)
	e^-	Gerjuoy & Stein (1955)
		Ehrhardt et al. (1968)
		England, Elford & Crompton (1988)
		Yoon et al. (2008)
CO	H_2	Yang et al. (2010)
	He	Cecchi-Pestellini et al. (2002)
	H	Walker et al. (2015)
H_2O	H_2	Faure et al. (2007)
		Faure & Josselin (2008)
	He	Green, Maluendes & McLean (1993)
		Nesterenok (2013)
	H	Daniel et al. (2015)
	e^-	Faure & Josselin (2008)

Dynamics of dust particles

The system of equations for grain charge distribution:

$$\frac{\mathrm{d}}{\mathrm{dz}}(n_{\mathrm{g,Z}} u_{\mathrm{g,Z}}) = n_{\mathrm{g,Z+1}} J_{\mathrm{e}}(a, Z+1) + n_{\mathrm{g,Z-1}} \left[J_{\mathrm{ph}}(a, Z-1) + \sum_j J_{\mathrm{j}}(a, Z-1) \right] - n_{\mathrm{g,Z}} \left[J_{\mathrm{e}}(a, Z) + J_{\mathrm{ph}}(a, Z) + \sum_j J_{\mathrm{j}}(a, Z) \right]$$

$J_{\mathrm{ph}}(a, Z)$ – the rate of photoelectric effect (Weingartner, Draine, 2001);

$J_{\mathrm{e}}(a, Z)$ – accretion rate of electrons (Draine, Sutin, 1987);

$J_{\mathrm{j}}(a, Z)$ – accretion of ions (Draine, Sutin, 1987);

Dust grains are considered as test particles. Grain velocity in the shock is (Draine, 1980):

$$\vec{u}_{\mathrm{g,Z}} = (u_{\mathrm{i}} - u_{\mathrm{n}}) \frac{\beta}{1+\beta^2} \vec{e}_{\mathrm{x}} + (u_{\mathrm{i}} - u_{\mathrm{n}}) \frac{\beta^2}{1+\beta^2} \vec{e}_{\mathrm{z}} + u_{\mathrm{n}} \vec{e}_{\mathrm{z}}$$

$$\beta = \frac{a - 1 + \left[(a-1)^2 + 4ab\right]^{1/2}}{2b}, \quad a = \frac{9\pi}{128} \frac{m}{kT_{\mathrm{n}}} \left(\frac{ZeB}{c\sigma\rho_{\mathrm{n}}} \right)^2, \quad b = 1 + \frac{9\pi}{128} \frac{m}{kT_{\mathrm{n}}} (u_{\mathrm{i}} - u_{\mathrm{n}})^2$$

The rate of momentum transfer from grains to neutral particles due to gas-grain scattering

$$\mathcal{F}_{\mathrm{n,d}} = \sum_Z n_{\mathrm{g,Z}}\, \sigma_{\mathrm{g}}\, \rho_{\mathrm{n}}\, (u_{z\mathrm{g,Z}} - u_{\mathrm{n}}) \times \left[\frac{128}{9\pi} \frac{k_{\mathrm{B}} T_{\mathrm{n}}}{\mu_{\mathrm{n}}} + (\vec{u}_{\mathrm{g,Z}} - \vec{u}_{\mathrm{n}})^2 \right]^{1/2}$$

Elastic scattering of neutral atoms and molecules on ions and electrons

Momentum and energy transfer between two components of the gas α and β (Draine, 1986):

$$\vec{\mathcal{F}}_{\alpha,\mathrm{el.sc.}} = \frac{n_\alpha n_\beta m_\alpha m_\beta}{m_\alpha + m_\beta}\left(\frac{2k_\mathrm{B}T_\mathrm{r}}{\pi m_\mathrm{r}}\right)^{1/2}(\vec{v}_\beta - \vec{v}_\alpha)\, s^{-3}\exp\left(-s^2\right)\int_0^\infty dx\, x^2\sigma(v = xc_\mathrm{r})\exp(-x^2)\left(2xs\cosh(2xs) - \sinh(2xs)\right)$$

$$\mathcal{G}_{\alpha,\mathrm{el.sc.}} = \frac{n_\alpha n_\beta m_\alpha m_\beta}{(m_\alpha + m_\beta)^2}\left(\frac{8k_\mathrm{B}T_\mathrm{r}}{\pi m_\mathrm{r}}\right)^{1/2}\exp\left(-s^2\right) 2k_\mathrm{B}\Bigg[\left(\frac{T_\beta - T_\alpha}{s}\right)\int_0^\infty dx\, x^4\sigma(x)\exp\left(-x^2\right)\sinh(2xs) +$$
$$+\frac{m_\beta T_\alpha}{m_\mathrm{r}}\int_0^\infty dx\, x^3\sigma(x)\exp\left(-x^2\right)\cosh(2xs) - \frac{m_\beta T_\alpha}{2sm_\mathrm{r}}\int_0^\infty dx\, x^2\sigma(x)\exp\left(-x^2\right)\sinh(2xs)\Bigg]$$

$$m_\mathrm{r} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}, \quad T_\mathrm{r} = \frac{m_\alpha T_\beta + m_\beta T_\alpha}{m_\alpha + m_\beta}, \quad s = \frac{|\vec{v}_\alpha - \vec{v}_\beta|}{c_\mathrm{r}}, \quad c_\mathrm{r} = \left(\frac{2k_\mathrm{B}T_\mathrm{r}}{m_\mathrm{r}}\right)^{1/2}$$

Cross sections of elastic scattering:
ions on molecules H_2 – Flower (2000);
ions on atoms H, He – Osterbrock (1961);
electrons on H – Dalgarno et al. (1999);
electrons on He – Crompton et al. (1970);
electrons on H_2 – Yoon et al. (2008);

Sputtering of icy mantles of dust grains

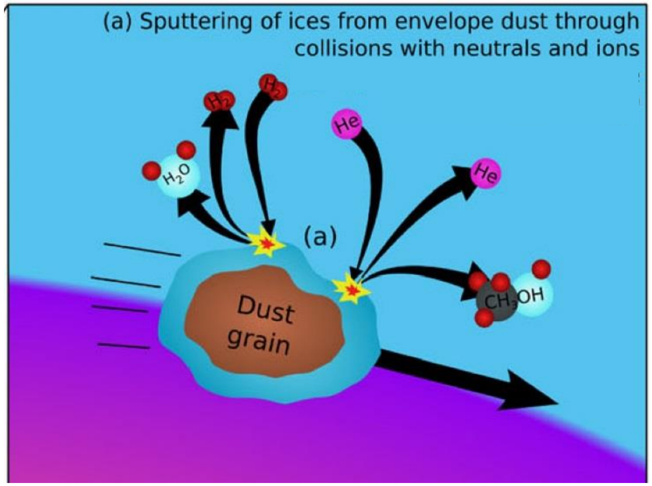
In the shock, icy mantles of grains are evaporated or sputtered in the gas-grain collisions.

$$k_{\mathrm{sp,j}} = \frac{\langle Y u\rangle_{\mathrm{jk}} n_{\mathrm{k}}}{4 N_{\mathrm{act}} N_{\mathrm{s}}} \quad [\mathrm{s}^{-1}]$$

$$\langle Y u\rangle_{\mathrm{jk}} = \left(\frac{8 k_{\mathrm{B}} T_{\mathrm{n}}}{\pi m_{\mathrm{k}}}\right)^{1/2} \frac{\exp(-\mathrm{s}^2)}{s} \times \int_0^\infty \mathrm{dx}\, \langle \mathrm{Y(x)}\rangle_{\theta,\mathrm{jk}}\, \mathrm{x}^2 \sinh(2\mathrm{xs}) \exp(-\mathrm{x}^2)$$

$$x = \sqrt{\frac{E}{k_{\mathrm{B}} T_{\mathrm{n}}}}, \quad s^2 = \frac{m_{\mathrm{k}} \left(\mathbf{u}_{\mathrm{g}} - \mathbf{u}_{\mathrm{n}}\right)^2}{2 k_{\mathrm{B}} T_{\mathrm{n}}}$$

$\langle Y(E)\rangle_{\theta,\mathrm{jk}}$ – average number of sputtered particles j per incident particle k. The sputtering yields were calculated according to Draine & Salpeter (1979).



(Suuterinen et al., 2014)

As a result, there is a system of differential equations for velocities and temperatures of neutral species, ions and electrons; chemical specimen concentrations; level population densities of atoms and molecules; charge distribution of dust grains – about 1100 equations. The differential equation solver CVODE v2.9.0 was used.

Modelling of the chemical evolution of dark cloud

The objectives of the modelling of 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.

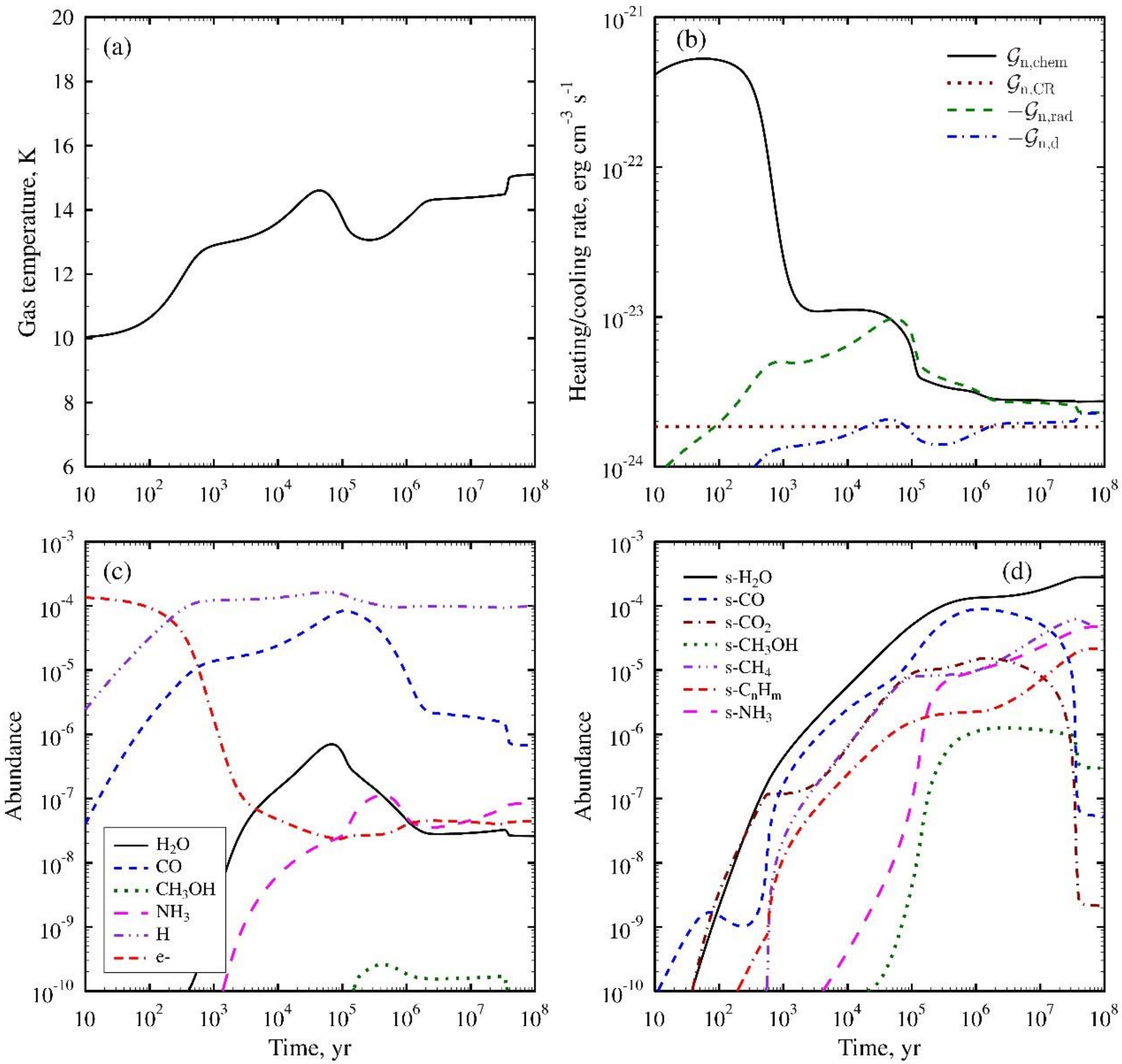
Initial chemical composition of the gas (Hincelin et al. 2011):

Species	Abundances
H_2	0.5
He	0.09
N	6.2×10^{-5}
O	2.8×10^{-4}
C^+	1.4×10^{-4}
S^+	8×10^{-8}
Si^+	8×10^{-9}
Fe^+	3×10^{-9}
Na^+	2×10^{-9}
Mg^+	7×10^{-9}
Cl^+	10^{-9}

Parameters of dark cloud

Parameter	Value
Gas density, $n_{\mathrm{H,tot}}$	2×10^4 cm^{-3}
Magnetic field strength, B_0	0.15 mG
Visual extinction, A_{V}	10
Micro-turbulence speed, v_{turb}	0.2 km s^{-1}
Velocity gradient	1 km s^{-1} pc^{-1}
Cosmic ray ionization rate, ζ	3×10^{-17} s^{-1}
Scaling factor of local interstellar radiation, G_0	1
Dust–gas mass ratio	0.01
Grain radius, a	0.1 μm
Grain material density	3.5 g cm^{-3}
Grain surface area density	4.8×10^{-22} cm^2 per H
Ortho-/para-H_2 ratio	1

Results. Chemical and thermal evolution of the dark cloud



(a) gas temperature;

(b) rates of main heating and cooling mechanisms of the gas;

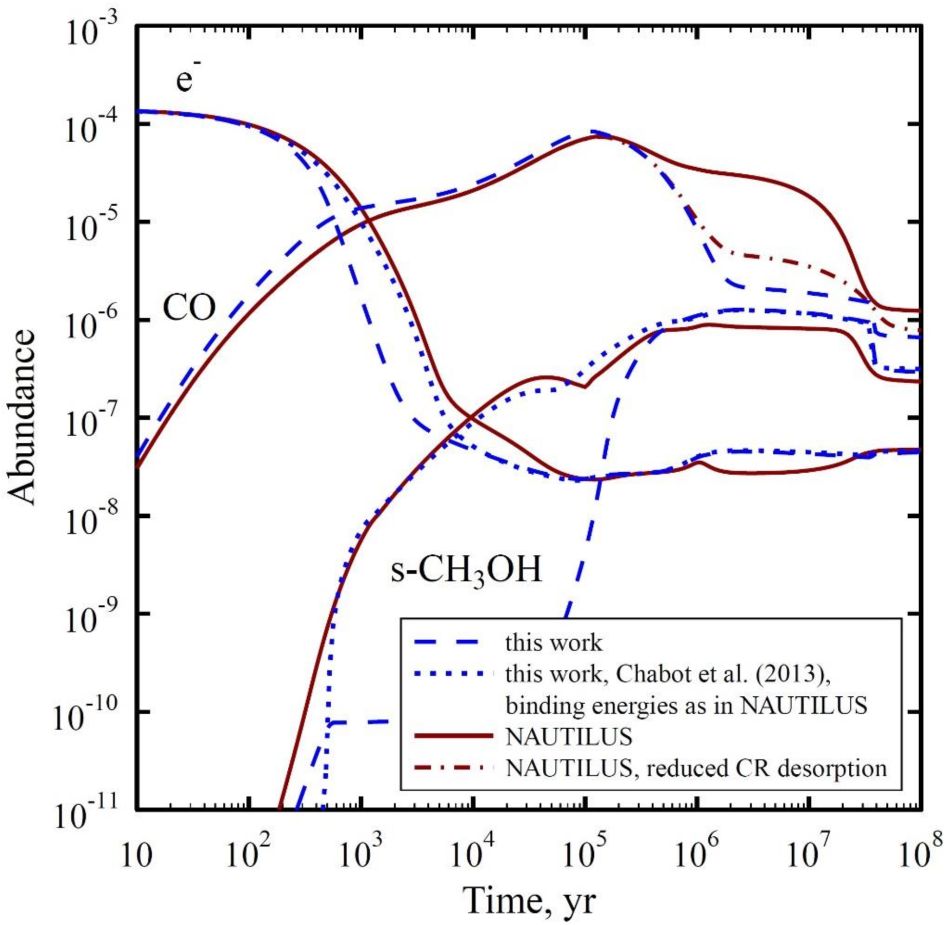
(c) abundances of gas species relative to hydrogen nuclei;

(d) abundances of grain mantle species.

Observational data, relative to H_2O ice (Boogert et al. , 2015):

Species	X_{H_2O}[a] [%]		
	MYSOs	LYSOs	BG Stars[c]
Securely identified species:[d]			
H_2O	100	100	100
CO	7	21	25
CO_2	19	28	26
CH_3OH	9	6	8

Comparison with NAUTILUS code



Models differ in

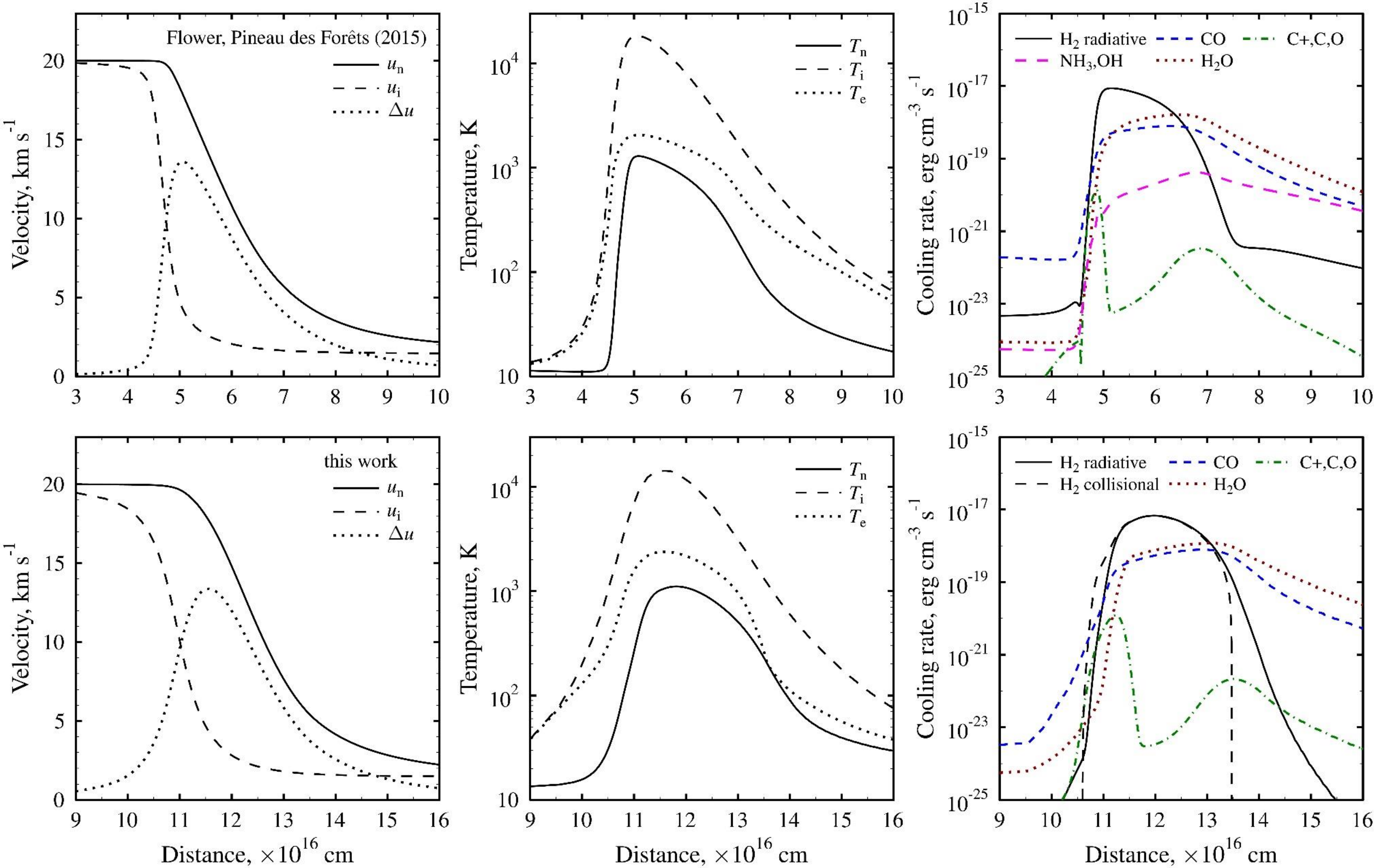
- networks for gas-phase chemical reactions – KIDA (is used in NAUTILUS) and UdfA (is used here);
- data on binding energies of chemical species on grain surface;

Chabot et al. (2013) presented set of branching ratios for chemical reactions:

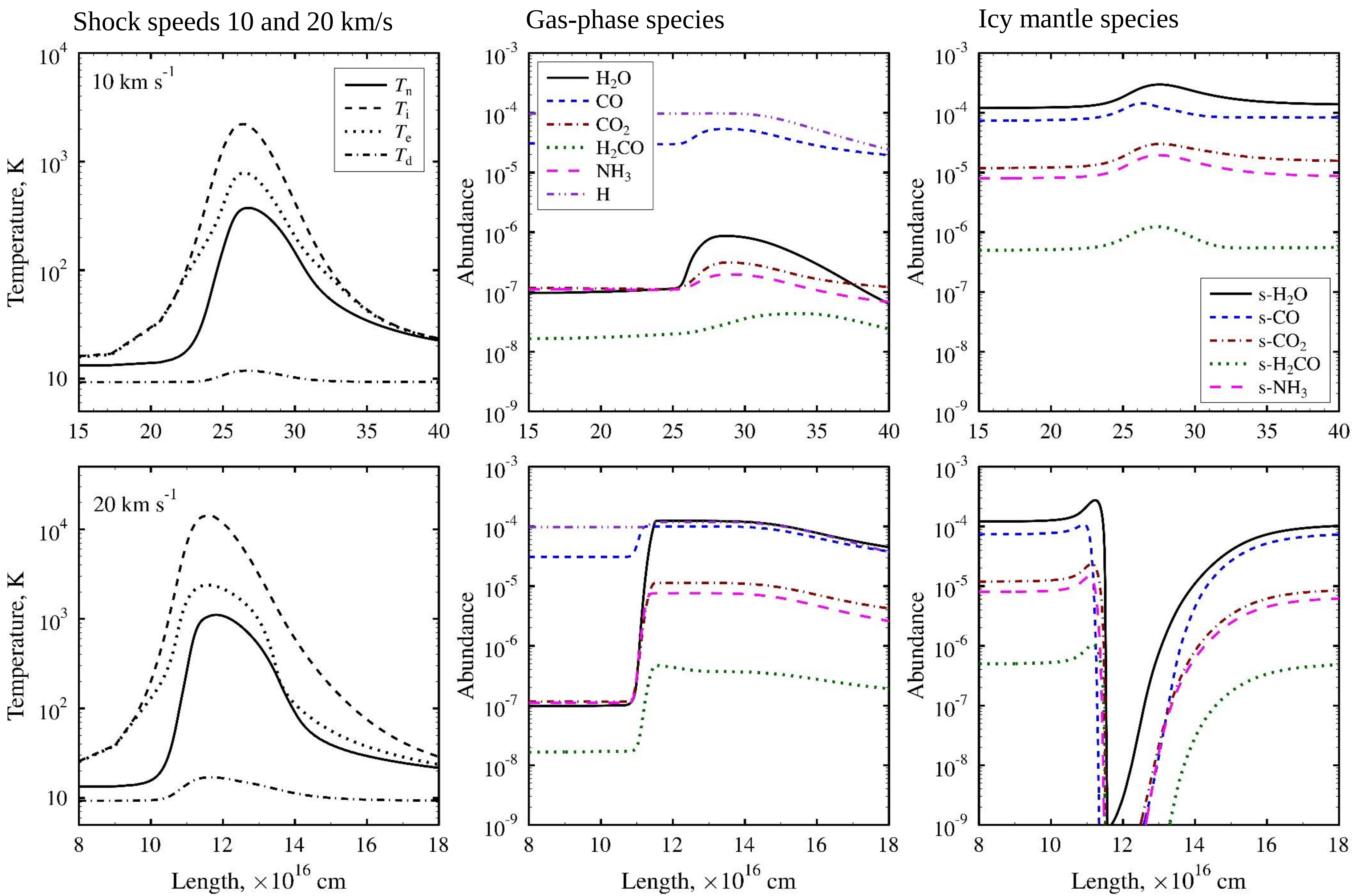
$$\mathrm{C_n}^- + \mathrm{C}^+ \rightarrow \mathrm{C_k} + \mathrm{C_l} + \mathrm{C_m}$$

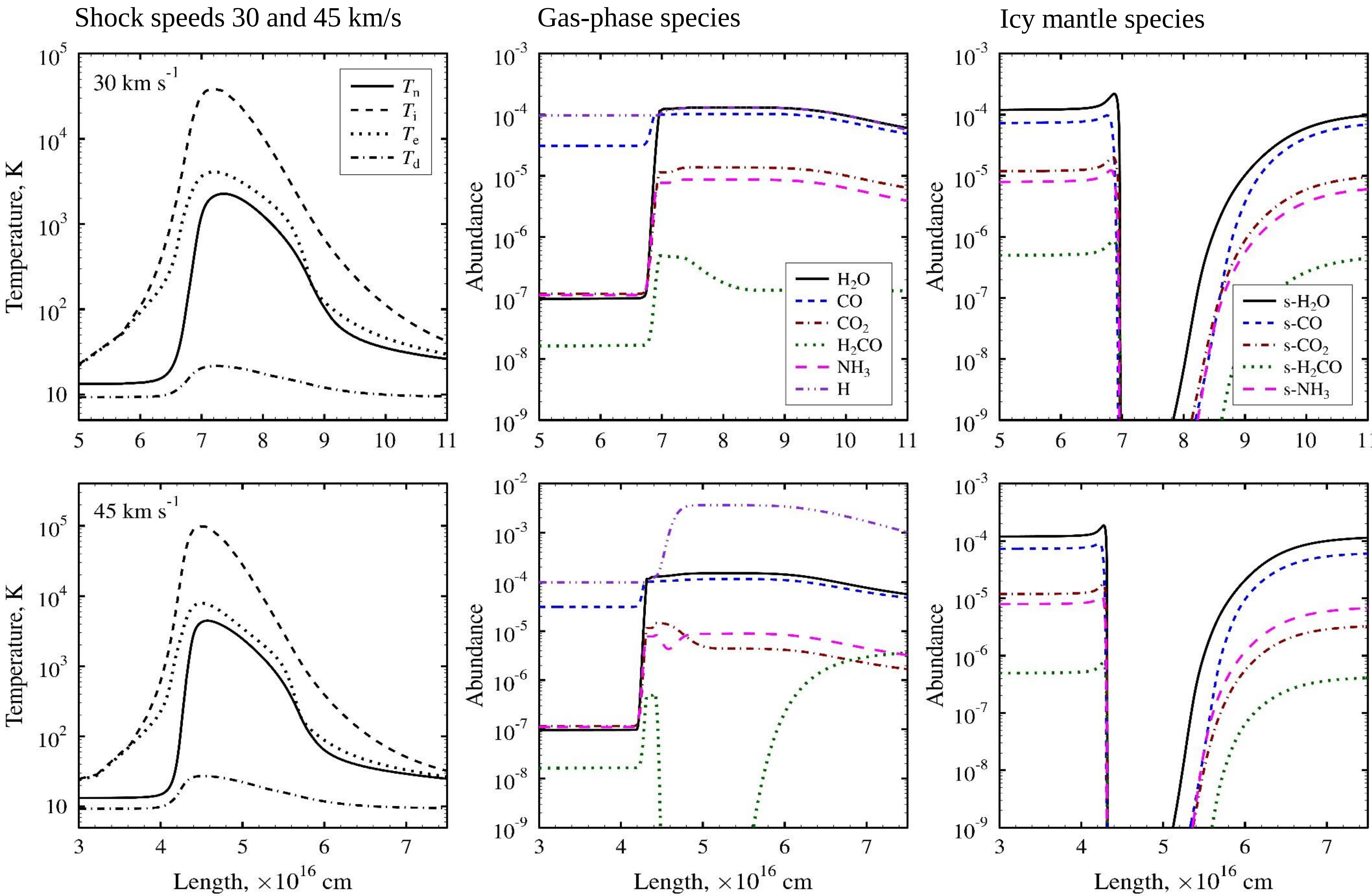
The figure shows the results of simulations with updated chemical network according to Chabot et al. (2013) and using the data on specimen binding energies as in NAUTILUS model. The results of NAUTILUS model with direct cosmic ray desorption reduced by an order of magnitude are shown.

Shock model results.
Comparison with the model by Flower & Pineau des Forets (2015)



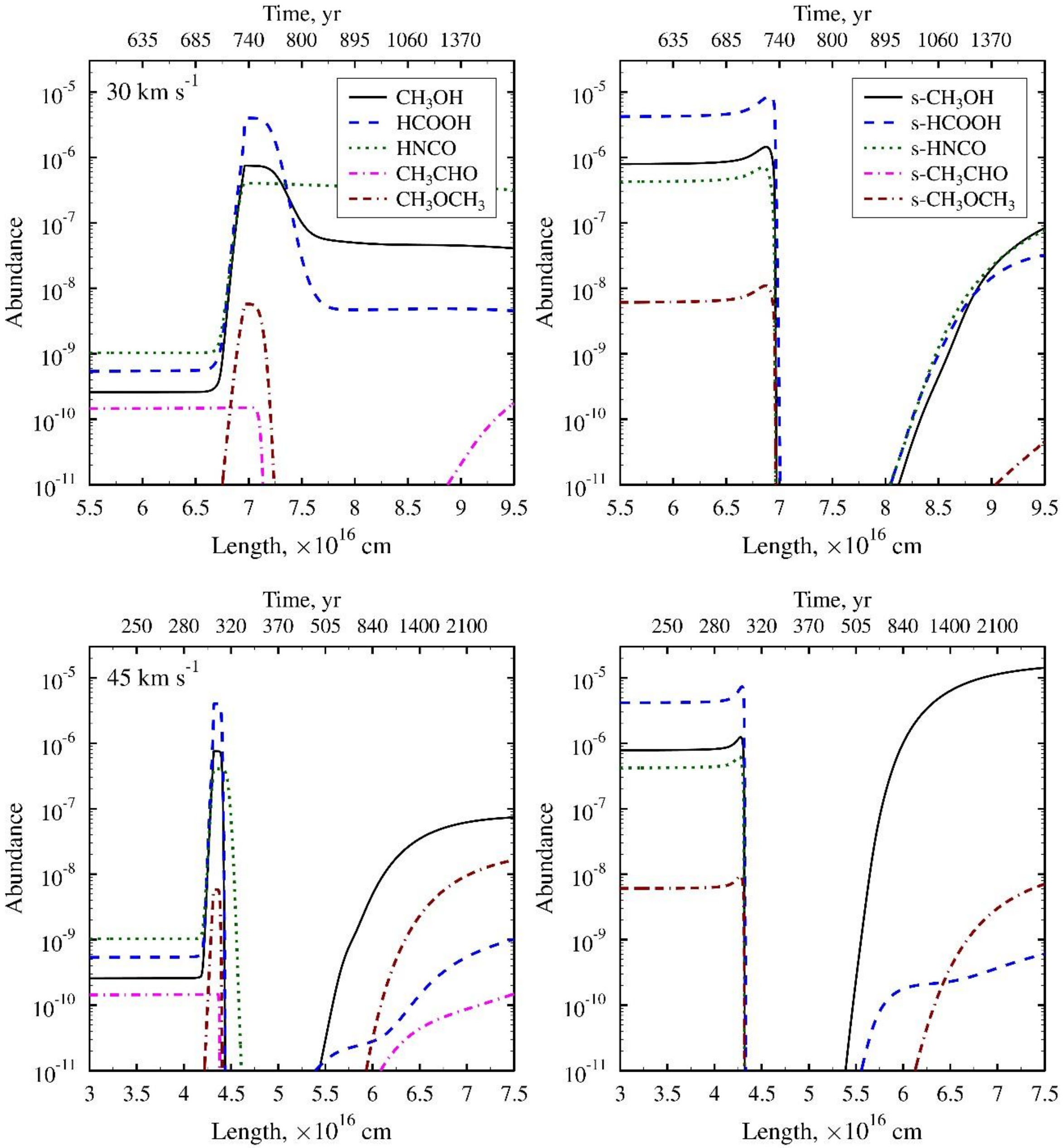
Chemical evolution of gas in the shock: simple species





Shock speeds 30 and 45 km/s
Gas-phase species
Icy mantle species
30 km s-1
45 km s-1
T_n
T_i
T_e
T_d
Temperature, K
Abundance
H_2O
CO
CO_2
H_2CO
NH_3
H
s-H_2O
s-CO
s-CO_2
s-H_2CO
s-NH_3
Length, $\times 10^{16}$ cm

Complex organic molecules (COMs)



Complex organic molecule (COM) – molecule with ≥ 6 atoms.

The COMs destroyed in the hot shocked gas could be reformed in the postshock region. The high abundance of simple species and radicals that are produced in the shock is one of the factors that promote COM production in the postshock gas.

The chemical network used in our model is incomplete for proper modelling of chemistry of COMs and extensions of gas-phase and grain surface chemistries must be used in the future work (Garrod 2013; Taquet et al. 2016; Fedoseev et al. 2017).

Conclusions

The chemical evolution of the gas in C-type shock wave is considered. The main results of the paper are summarized below:

(i) The time-scale for molecule survival in the high-velocity shock is low – of the order of dozens of years.

(ii) For high-speed shocks, $u_s \geq$ 40-45 km/s, the abundance of H atoms and radicals in the postshock gas is relatively high, that affects the gas-phase and grain surface chemistries.

(iii) At high shock speeds, the postshock abundances of some COMs such as methyl formate may be much higher than in the preshock gas due to efficient gas-phase production.

(iv) The shock model presented can be employed to interpret observational data on molecular emission from protostellar outflows, to study formation of biologically relevant molecules in shock regions, and can be also used for modelling of cosmic masers.

Recent models of C-type shocks

1. The model by Flower & Pineau des Forets (2015)
The solution of magnetohydrodynamic equations, calculation of population densities of molecules and atoms, gas-phase chemistry, adsorption of gas-phase species on dust and dust sputtering.

2. The model by Palau et al. (2017)
The parametric model of shock (MHD equations are not solved, approximate formulas for shock profile are used). Complete gas-phase and grain surface chemistries.

3. The model by Holdship et al. (2017)
The parametric model of shock. Complete gas-phase and grain surface chemistry, sputtering of icy mantles.

4. The model by Burkhardt & Herbst (in prep.)
The parametric model of shock coupled to the astrochemical code NAUTILUS.

The main motivation is to investigate the chemical processing of complex molecules, e.g. relevant for the life genesis, in the star formation process.