Modelling non-dissociative shock waves in interstellar medium: first results

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Abstract.
The structure of steady one-dimensional shock waves in partially ionized interstellar gas is studied. The model is constructed of so called C-type shocks where the physical parameters characterizing the flow change continuously at the shock front. We present our first results of the modelling of C-type shocks. The model will be employed to study molecular line emission from interstellar shocks, in particular, maser emission.

1. Introduction
Interstellar shock waves play a major role in the chemical and physical evolution of the interstellar medium. These shocks result from the expansion of HII regions, cloud-cloud collisions, stellar winds, supernova explosions [1].

The nature and structure of interstellar shocks are strongly dependent upon the strength and orientation of the magnetic field and the local ionization fraction in the pre-shock gas [2, 3]. For strong transverse magnetic fields or low shock velocities, magnetosonic waves can propagate faster than the shock front forming a magnetic precursor to the shock. The ionized fluid is accelerated and heated by the magnetic precursor. The resulting drift between the ionized and neutral fluids heats and accelerates the neutral component of the gas. Due to ion-neutral scattering the discontinuity in the neutral fluid can then disappear – a C-type, or ‘continuous’, shock forms. If the temperature of the neutral gas is low enough due to molecular and atomic cooling, the neutral gas remains supersonic everywhere within the shock. In C-type shocks, molecules are at most partially dissociated. Therefore, a characteristic feature of C-type shocks is strong molecular emission.

The intent of the present paper is to discuss the general properties of C-type magnetohydrodynamic shock waves.

2. Shock wave model
2.1. Magnetohydrodynamic equations
A steady, one-dimensional flow along the z-direction is considered. The magnetic field \( B_0 \) is adopted to be transverse to the flow direction. The flow components considered are neutrals, ions, and electrons, denoted by subscripts \( n, i \), and \( e \), respectively. Each component is assumed to have velocity \( v(z) \), density \( \rho(z) \), and temperature \( T(z) \), with the condition of stationarity \( \partial v/\partial t = \partial \rho/\partial t = \partial T/\partial t = 0 \). Electrons and ions are assumed to move at the same velocity [2].
The fluid equations that express conservation of particle number density, mass, momentum, and energy are [3]:

\[
\begin{align*}
\frac{d}{dz} \left[ \frac{\rho n v_n}{\mu n} \right] &= N_n \quad (1) \\
\frac{d}{dz} \left[ \frac{\rho i v_i}{\mu i} \right] &= N_i \quad (2) \\
\frac{d}{dz} [\rho n v_n] &= S_n \quad (3) \\
\frac{d}{dz} [\rho i v_i] &= -S_n \quad (4) \\
\frac{d}{dz} \left[ \rho n v_n^2 + kT n \frac{\rho n}{\mu n} \right] &= F_n \quad (5) \\
\frac{d}{dz} \left[ \rho i v_i^2 + kT i \frac{\rho i}{\mu i} + kT e n_e v_i + \frac{B_0^2 v_i^2}{8\pi v_i^2} \right] &= -F_n \quad (6) \\
\frac{d}{dz} \left[ \frac{1}{2} \rho n v_n^3 + \left( \frac{5}{2} kT n + U_n \right) \frac{\rho n}{\mu n} v_n \right] &= G_n + F_n v_n - \frac{1}{2} S_n v_n^2 \quad (7) \\
\frac{d}{dz} \left[ \frac{1}{2} \rho i v_i^3 + \frac{5}{2} kT i \frac{\rho i}{\mu i} v_i + \frac{5}{2} kT e n_e v_i + \frac{B_0^2 v_i^2}{4\pi v_i} \right] &= G_i + G_e - F_n v_i + \frac{1}{2} S_n v_i^2 \quad (8) \\
\frac{d}{dz} \left[ \frac{3}{2} kT i \frac{\rho i}{\mu i} v_i - \frac{3}{2} kT e n_e v_i \right] + \left[ kT i \frac{\rho i}{\mu i} - kT e n_e v_i \right] \frac{dv_i}{dz} &= G_i - G_e \quad (9)
\end{align*}
\]

where \(v_s\) is the shock speed, \(\mu_n\) is the mean mass per neutral particle and \(\mu_i\) is the mean mass per ion particle; \(U_n\) is the mean internal energy per neutral particle. The source terms \(N_n, N_i, S_n, F_n, G_n, G_i\) and \(G_e\) have the following definitions: \(N_n\) and \(N_i\) are the numbers of neutral particles and ions created per unit volume and time as a result of chemical reactions; \(S_n\) is the rate per volume at which ion-electron mass is converted into neutral mass; \(F_n\) is the rate per volume at which momentum is transferred from the charged fluid to the neutral fluid as a result of elastic scattering and chemical reactions; \(G_n, G_i\) and \(G_e\) are the rates, per volume, at which thermal energy is added to the neutral, ion and electron fluids, respectively.

2.2. Ion-neutral elastic scattering
Momentum exchange between neutral and charged fluids occurs through ion-neutral elastic scattering and by collisions of neutral particles with charged dust grains. The momentum transfer cross sections for the scattering of ions and neutral particles (H, He, H\(_2\)) were calculated using the results by [4]. For the elastic scattering between electrons and neutral particles, the momentum transfer cross sections were adopted from [5–7]. The rates of momentum transfer and gas heating due to elastic scattering were calculated according to [8] using the given dependence of the cross section on velocity.

The expression for energy transfer between ions and electrons was taken from [9].

2.3. Chemistry
The UMIST database for astrochemistry [10] was used in our simulations. The chemical species containing atoms H, He, C, N, O, Na, Mg, Si, S, Cl, Fe were taken into account.
The total number of gas species is 426. We took into account gas-phase chemical reactions, direct cosmic-ray ionization, cosmic-ray-induced photoreactions, photoreactions induced by interstellar background ultraviolet (UV) field, adsorption of neutral species on grains and various desorption mechanisms [11, 12]. The rates of endothermic reactions between ions and neutrals were calculated by the method of 'effective' temperature [2].

The differential equations for the concentrations of chemical species were solved together with the magnetohydrodynamic equations.

2.4. Calculation of molecule level populations
The energy level populations of H₂, CO and H₂O molecules were computed in parallel with dynamical and chemical rate equations. We took into account 150 ro-vibrational levels for each of molecules H₂, ortho- and para-H₂O and 41 levels of ground vibrational state of CO molecule. Spectroscopic data were taken from [13, 14] for H₂ molecule and from HITRAN 2012 database [15] for CO and H₂O molecules. Rate coefficients for collisions of H₂ molecule with He, H₂ and H were taken from [16–21]. For collisions of H₂ with thermal electrons, rate coefficients were calculated using the recipes given by [22, 23]. We took into account the excitation of ro-vibrational levels of H₂ molecule in collisions with fast electrons produced by cosmic ray ionization of the gas [24]. Rate coefficients for collisions of CO with He, H₂, H were taken from [25–27]. Information on H₂O collision data used in calculations can be found in [28].

Level populations of ions CI, CII and OI were computed. The excitation of atomic levels by H₂, He, H and thermal electrons was taken into account [29]. The large velocity gradient approximation was used in calculations of radiative transition probabilities of molecular and atomic species [30]. The dust radiation was neglected in these calculations.

The system of differential equations was solved using the computer program CVODE v2.8.2, which is available in the web [31].

2.5. Gas cooling
We took into account cooling of gas via excitation of fine structure transitions of ions (OI, CI and CII) and ro-vibrational lines of molecules (H₂, CO and H₂O).

2.6. Dust model
A simple single-size grain model was adopted in the calculations. The grain radius was assumed to equal 0.1 µm and the dust-gas mass ratio is equal to 0.01. The grains were assumed to compose from carbonaceous material [32]. We considered the heating of dust by diluted star light and UV interstellar background, by collisions with gas species, by gas species adsorption, and H₂ molecule formation. The photoelectric emission from dust grains, the electron attachment and ion recombination were taken into account. Reaction rates were calculated according to [33]. Reactions of neutralization and dissociative neutralization of ions on grain surface were considered [34]. Dust grain dynamics was treated according to [2]. The momentum transfer between neutral particles and charged grains was taken into account.

2.7. UV field
We used the average local interstellar UV field approximated by [35]. The interstellar radiation field is reduced in accordance with visual extinction. We took into account the UV field generated internally via excitation and fluorescence of electronic states of H₂ molecules in the process of cosmic ray propagation through the gas [36].
### Table 1. Parameters of the molecular cloud

| Parameter                                      | Value                        |
|------------------------------------------------|------------------------------|
| Total H concentration, \( n_H \)              | \( 2 \times 10^4 \text{ cm}^{-3} \) |
| Visual extinction, \( A_V \)                  | 10                           |
| Cosmic ray ionization rate, \( \zeta \)       | \( 10^{-16} \text{ s}^{-1} \)  |
| The ratio of visual extinction to reddening, \( R_V \) | 5.5                         |
| Transverse magnetic field, \( B_0 \)          | 0.1 mG                       |
| Grain surface area, \( S_g \)                 | \( 7.8 \times 10^{-22} \text{ cm}^2/\text{H} \) |

### 3. Results

#### 3.1. Chemical evolution of stationary molecular cloud

Parameters of a molecular cloud are given in the table 1. The chemical and thermal evolution of the stationary cloud was calculated, starting with some arbitrary initial values of specimen concentrations and gas temperature. We took low metal elemental abundances that are expected to reproduce the gas-phase chemistry of dense cold clouds [34]. All metal atoms with the exception of O and N, are in ionic state in the adopted initial chemical abundances.

The calculation results are shown in the figure 1. It is seen that the gas reaches thermal equilibrium after about \( 10^4 \) years. A small decrease of the gas temperature at about several \( 10^3 \) years comes from the increase of \( \text{H}_2\text{O} \) and \( \text{CO} \) concentrations and, hence, increase of gas cooling. The temperature of the gas remains at relatively constant level close to 20 K until approximately \( 10^6 \) years. After this time, the effect of molecule depletion from the gas phase becomes significant – main coolants \( \text{H}_2\text{O} \) and \( \text{CO} \) become adsorbed on dust grains and the temperature of the gas rises. According to our results, the dominant O-bearing specimen at the end of the chemical evolution is \( \text{CO} \) molecule. Carbon monoxide is effectively produced in the gas, while the production of \( \text{H}_2\text{O} \) is not effective at low gas temperatures. The ionization fraction of the gas is low, of the order \( 10^{-7} \). The total charge carried by dust grains is negligibly small compared to the electron concentration.

For simulations of shock waves, the chemical composition and temperature of the gas at \( 5 \times 10^5 \) years were taken.

#### 3.2. C-type shock wave

Figure 2 presents simulation results for the C-type shock of speed 20 km/s. The results are consistent in general with previous studies of C-type shocks [3]. The scattering of gas molecules on charged grains is the dominant mechanism of the momentum transfer from the charged fluid to the neutral gas at gas densities in question. Consequently, simulation results are sensitive to the assumed dust properties such as specific surface area. Two velocity dependences of cross section for \( \text{H}_2 \)-ion elastic scattering were considered: (i) the cross section is inversely proportional to the relative velocity and (ii) the cross section dependence found by [4]. The shock width is almost insensitive to the form of the cross section dependence on velocity of ion-neutral scattering. According to our calculations, the electron temperature is much lower than the ion temperature. The excitation of ro-vibrational levels of \( \text{H}_2 \) is very effective cooling mechanism of electron fluid [3].

Some important physical effects such as grain mantle sputtering are not yet included in our model. Grain mantle sputtering releases molecules to the gas phase which can significantly modify cooling rate of the gas.
Figure 1. Chemical evolution of a dark cloud; (a) concentrations of chemical species; (b) gas temperature.

Figure 2. Results of C-type shock wave calculations. The steady-state profiles of (a) velocity, (b) temperature.

4. Conclusions
The model of the C-type shock in interstellar cloud is presented. Simulation results are consistent in general with previous studies. Important physical effects such as sputtering of grain mantles are not yet included in our model.
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