Astrochemistry in the Orion BN-KL region

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Abstract

Massive and young stars inside populated clusters can suffer close dynamical encounters leading to energetic and explosive events. Evidence suggests that Orion BN-KL, at 414 pc, suffered a dynamical decay 500 years ago. This region shows one of the highest diversity of molecular abundances and a filamentary structure known as Orion fingers.

In this work we propose a Newton-Rhapson method to solve the kinetic chemical reactions of 31 chemical species using the reaction coefficients in the UMIST database [3]. We have tested this method using a dark cloud with homogeneous density and 10 K temperature and the relative abundances are compared to the UMIST database results.

Aims

- Analyze observations of Orion BN/KL
- Program an algorithm of reaction selection
- Solve a chemical network of species and reactions
- Implement the chemistry network solution into a hydrodynamic solver
- Calculate the total cooling according to the network
- Compare simulations to observations

Reaction equations

$$\frac{dn_i}{dt} = \sum_{species} formation - \sum_{species} destruction, \tag{1}$$

$$\frac{dn_i}{dt} = \sum_{j,k} k_{jk} n_j n_k + \sum_{l} k_l n_l - n_i \left[\sum_{m} k_{im} n_m + \sum_{n} k_n \right], \tag{2}$$

$$\frac{dn_l}{dt} = R_l, \qquad Q_l = \frac{\Delta n_l}{\Delta t} - R_l, \qquad Q_l = 0, \tag{3}$$

with $l = 1, 2, ..., p$ and $p < N$ where N is the total of species.

Conservation equations

$$A_T = \sum^{species} k \cdot A_k \cdot B_l, \tag{4}$$

then,

$$C_m = A_T - \sum_{k}^{species} k \cdot A_k \cdot B_l, \tag{5}$$

$$C_m = 0, \tag{6}$$

para $m = p + 1, p + 2, ..., N$.
The root $Q_l = 0$ and $C_m = 0$ are needed and this can be written as

$$\mathbf{Q} = \left[Q_1, \quad ..., \quad Q_p, \quad C_{p+1}, \quad ..., \quad C_N \right] = 0. \tag{7}$$

UMIST

UMIST database (McElroy et al. 2013) contains the gas chemistry descibed by 6173 reactions between 467 species (268 cations, 28 anions and 171 neutral species) formed with 13 elements. This network includes a code, Rate12, to solve the differential equations.

Table : UMIST Format

RN.:type:R1:R2:P1:P2:P3:P4:NE:[α:β:γ:T_l:T_u:ST:ACC:REF]

Heading	Description
type	Reaction type
α, β, and γ	Parameters to calculate reaction rate coefficients
T_l/T_u	Lower/upper temperature

Reaction types

- Two body

$$k = \alpha(T/300)^{\beta} \exp(-\gamma/T) \quad [\mathrm{cm^3 s^{-1}}], \tag{8}$$

- Direct cosmic ray ionisation

$$k = \alpha \quad [\mathrm{s^{-1}}], \tag{9}$$

- Cosmic rays induced

$$k = \alpha(T/300)^{\beta} \frac{\gamma}{1-\omega} \quad [\mathrm{s^{-1}}], \tag{10}$$

- Photons

$$k = \alpha \exp(-A_v \gamma) \quad [\mathrm{cm^3 s^{-1}}], \tag{11}$$

Newton-Raphson

$$\mathbf{Q}(\mathbf{n}_0 + \Delta\mathbf{n}) = \mathbf{Q}(\mathbf{n}_0) + \sum_{j=1}^{N} \frac{\partial Q_i}{\partial n_i} \Delta\mathbf{n}_j + O(\Delta\mathbf{n}^2) \tag{12}$$

$$\mathbf{Q}(\mathbf{n}_0) + \mathbf{J} \cdot \Delta\mathbf{n}_j = 0 \Longrightarrow \mathbf{n} = \mathbf{n}_0 - \mathbf{J}^{-1}\mathbf{Q}(\mathbf{n}_0) \tag{13}$$

$$\mathbf{n}_{i+1} = \mathbf{n}_i - \mathbf{J}^{-1}(\mathbf{n}_i)\mathbf{Q}(\mathbf{n}_i) \tag{14}$$

Initial guess

$$\zeta' = min\left[\frac{A_T}{k}, \frac{B_T}{l}\right]$$
$$\zeta = \zeta'/2.$$

Convergence factor

$$f = \left(\frac{N_{it} - n}{N_{it}}\right)^{\gamma}$$

Resolution.

$$\frac{|n_l^k - n_l^{k+1}|}{n_l^{k+1}} < \epsilon\,,$$

KIMI

Acuchem (Braun et al. 1988) was compared to KIMI in the system:

$$a \rightarrow b, \qquad b \rightarrow c, \qquad c \rightarrow d, \tag{15}$$

$$k_1 = 0.1 \quad [\mathrm{s}^{-1}] \qquad k_2 = 0.2 \quad [\mathrm{s}^{-1}] \qquad k_3 = 0.12 \quad [\mathrm{s}^{-1}]. \tag{16}$$

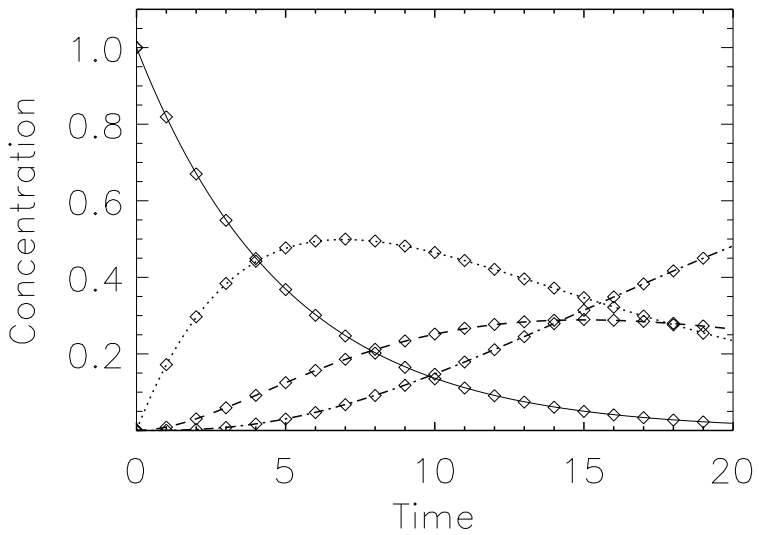


Figure : Acuchem, in rhombus, and KIMI for a, b, c y d in solid line, dotted line, dashed line y dot-dashed line, respectively.

Dark Cloud

Let's use an isotropic and homogeneus object to model a dark cloud with $n(\mathrm{H_2}) = 10^4$ cm^{-3}, T=10 K, $A_v = 10$ mag, albedo $\omega = 0.6$ and a cosmic ray ionisation rate of 1.3 $\times 10^{-17}$ s^{-1}.
The only relevant reaction to form H_2 is between 2 H atoms in the surface of dust grains

$$\frac{dn_{\mathrm{H_2}}}{dt} = 5.2 \times 10^{-17} \left(\frac{T}{300}\right)^{0.5} n_H n(H) \quad [\mathrm{cm^{-3}\,s^{-1}}] \qquad (17)$$

Species i	n_i/n_{H}	Species i	n_i/n_{H}
H_2	0.5	H	5.0×10^{-5}
C	1.4×10^{-4}	O	3.2×10^{-4}

Table : Initial conditions used in KIMI

Dark Cloud: CO

Table : Relative abundances in a dark cloud with 13 species and 10^8 yr

Especie	Density $\log(X/H_2)$ KIMI	Rate12	Specie	Density $\log(X/H_2)$ KIMI	Rate12
H	-3.60	-3.60	C	-4.42	-8.43
H+	-4.91	-10.02	C2	-17.00	-12.43
CH	-9.96	-10.47	O	-3.55	-3.54
CH2	-3.95	-11.33	O2	-4.03	-4.19
H2O	-4.33	-6.35	HCO	-17.00	-11.25
OH	-7.93	-7.49	CO2	-7.08	-6.94
CO	-3.88	-3.55			

- Only hydrogen can be ionised.
- H, C y O are the only elements in the network and there's a limit of 3 atoms per molecule.
- 140 reactions

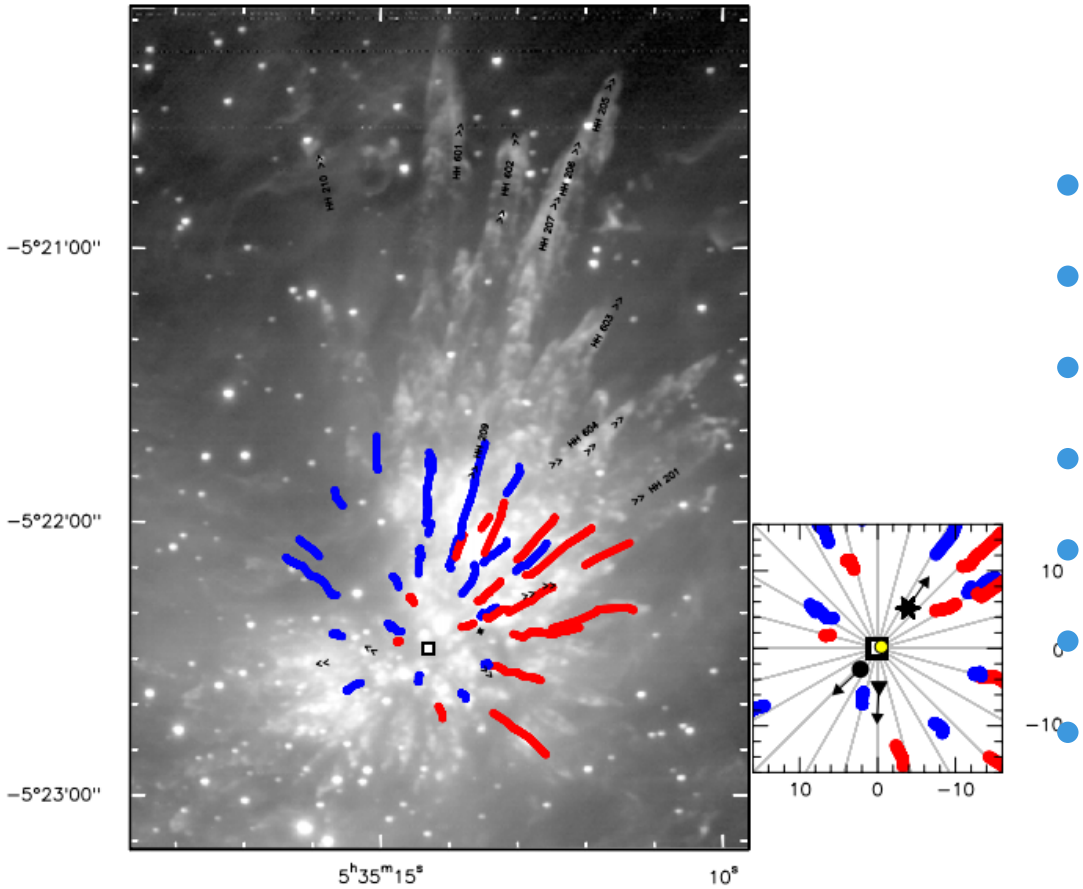
Dark Cloud: 31 species

Table : Relative abundances in a dark cloud with 31 species and 10^8 yr

Especie	Density $\log(X/H_2)$ KIMI	Rate12	Specie	Density $\log(X/H_2)$ KIMI	Rate12	Specie	Densidad $\log(X/H_2)$ KIMI	Rate12
C	-6.85	-8.43	CH_3	-7.88	-11.33	O_2H	-29.34	-12.62
C_2	-14.60	-12.43	CH_4	-13.38	-6.91	H+	-6.09	-10.02
C_2H	-14.25	-11.23	CO_2	-9.54	-6.94	H-	-12.54	-12.81
C_2H_2	-13.73	-8.60	H	-3.65	-3.60	H2+	-12.24	-12.54
C_2O	-13.66	-12.91	H_2CO	-9.92	-11.20	H_3+	-8.42	-9.40
C_3	-13.37	-9.88	H_2O	-15.59	-6.35	H_2	0.00	4.30
C_3H	-42.00	-11.93	H_2O_2	-42.00	-19.32	CO	-3.55	-3.55
C_3O	-29.61	-9.80	HCO	-13.38	-11.25	OH	-10.36	-7.49
CH	-18.70	-10.47	O	-3.44	-3.64	e	-6.09	-7.47
CH_2	-42.00	-11.33	O_2	-7.88	-4.19			

- Only hydrogen can be ionised.
- H, C y O are the only elements in the network and there's a limit of 5 atoms per molecule.
- 240 reactions

Orion BN/KL



- Common center
- Explosive law
- Isotropy
- H_2 fingers
- CO fingers
- FeII Bullets
- $T = T_a \tan i$

Figure : Zapata, 2013

Formation

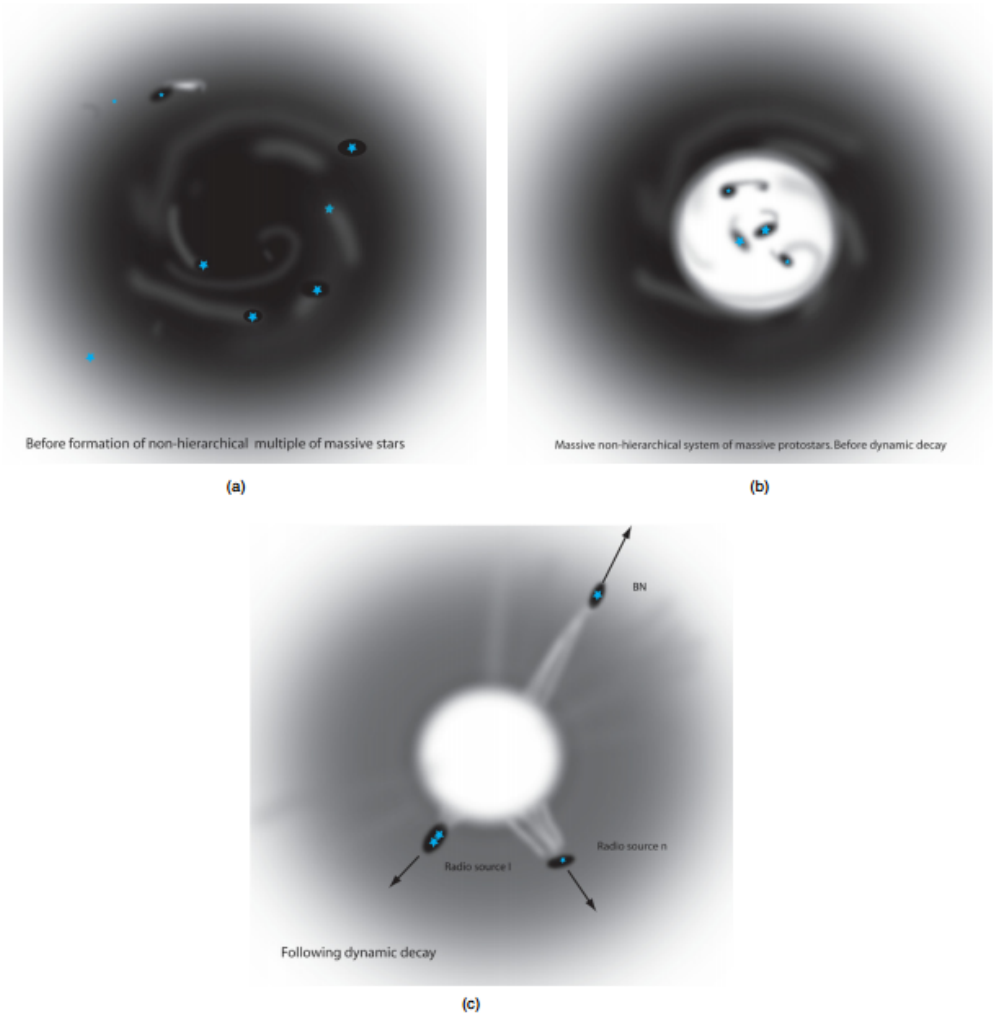


Figure : Orion BN-KL formation model (Bally, 2011)

Bally's model

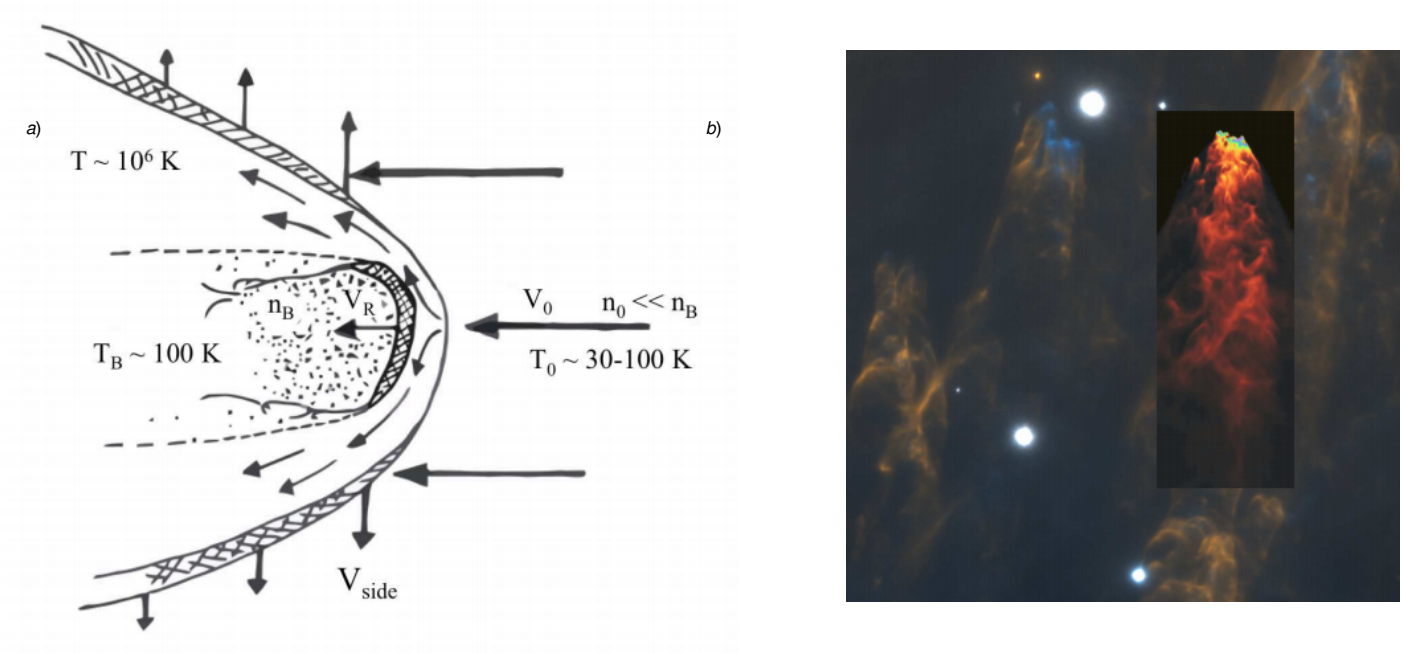


Figure : Finger formation model (Bally et al. 2015)

hydrodynamics

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = \mathbf{S} \tag{18}$$

$$\mathbf{U} = \left[\rho, \quad \rho\mathbf{v_x}, \quad \rho\mathbf{v_y}, \quad \rho\mathbf{v_z}, \quad \mathbf{E}, \quad \rho_l, \quad \rho_{l+1}, \quad \ldots \rho_{nspec}\right] \tag{19}$$

$$\mathbf{F} = \left[\rho\mathbf{v_x}, \quad \mathbf{P} + \rho\mathbf{v_x^2}, \quad \rho\mathbf{v_x}\mathbf{v_y}, \quad \rho\mathbf{v_x}\mathbf{v_z}, \quad \mathbf{v_x}(\mathbf{E}+\mathbf{P}), \quad \rho_l v_x, \quad \rho_{l+1} v_x, \quad \ldots, \rho_{nspec} v_x\right] \tag{20}$$

$$\mathbf{G} = \left[\rho\mathbf{v_y}, \quad \rho\mathbf{v_x}\mathbf{v_y}, \quad \mathbf{P} + \rho\mathbf{v_y^2}, \quad \rho\mathbf{v_y}\mathbf{v_z}, \quad \mathbf{v_y}(\mathbf{E}+\mathbf{P}), \quad \rho_l v_y, \quad \rho_{l+1} v_y, \quad \ldots, \rho_{nspec} v_y\right] \tag{21}$$

$$\mathbf{H} = \left[\rho\mathbf{v_z}, \quad \rho\mathbf{v_x}\mathbf{v_z}, \quad \rho\mathbf{v_y}\mathbf{v_z}, \quad \mathbf{P} + \rho\mathbf{v_z^2}, \quad \mathbf{v_z}(\mathbf{E}+\mathbf{P}), \quad \rho_l v_z, \quad \rho_{l+1} v_z, \quad \ldots, \rho_{nspec} v_z\right] \tag{22}$$

$$\mathbf{S} = \left[0, \quad 0, \quad 0, \quad 0, \quad \mathbf{G} - \mathbf{L}, \quad S_l, \quad S_{l+1}, \quad \ldots, S_{nspec}\right] \tag{23}$$

Cooling

$$L_M = n_{H_2}^2 x_M \Lambda_M \qquad \Lambda_M = \Lambda_M(T, n_{H_2}, N) \tag{24}$$

n_{H_2} is the H_2 density, $x_M = n_M/n_{H2}$ and Λ_M cooling coefficient. Also $N = N(n_{H_2})$ is an optical depth parameter.

$$\frac{1}{\Lambda_M} = \frac{1}{L_0} + \frac{n_{H_2}}{n_{1/2}} + \frac{1}{L_0}\left(\frac{n_{H_2}}{n_{1/2}}\right)^{\alpha}\left(1 - \frac{n_{1/2}L_0}{L_{LTE}}\right) \tag{25}$$

where L_0, L_{LTE}, $n_{1/2}$ y α are T and N functions.

- Diatomic hydride
  HCl
- Diatomic heteronuclear
  $\Lambda_M = \Lambda_{CO}(T, 0.01 n_{H_2}, 100N)$
- Poliatomic dihydride H_2O
- Poliatomic
  $\Lambda_M = \Lambda_{CO}(T, 0.008 n_{H_2}, 7N)$

Results

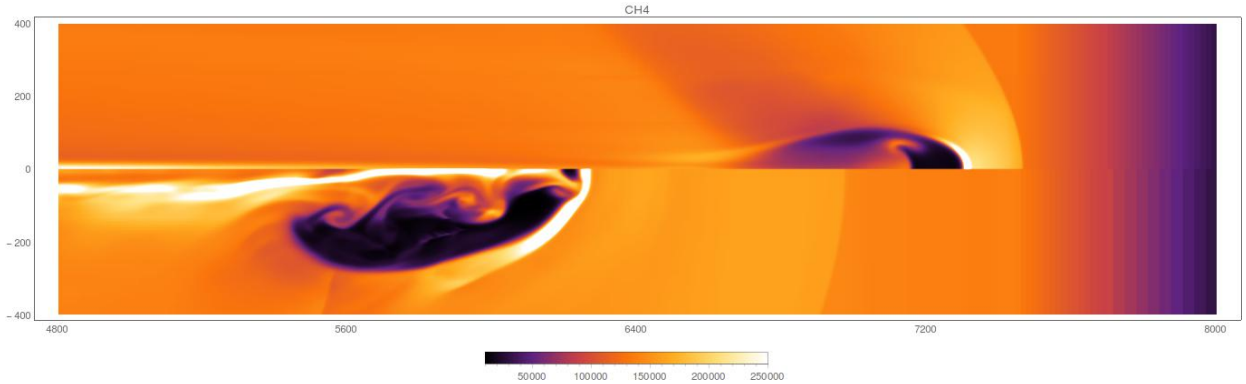


Figure : CH_4 structure at 135 and 180 years. ([cm^{-3}], [AU])

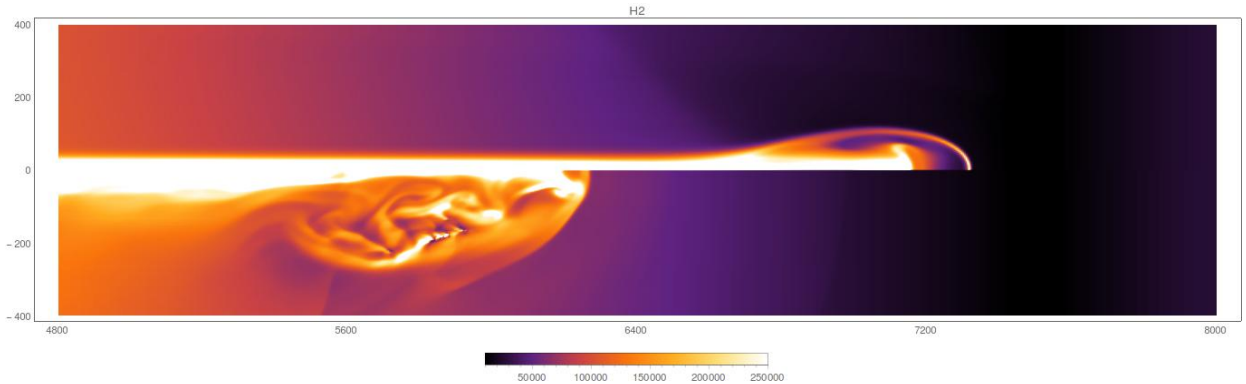


Figure : H_2 structure at 135 and 180 years. ([cm^{-3}], [AU])

Results

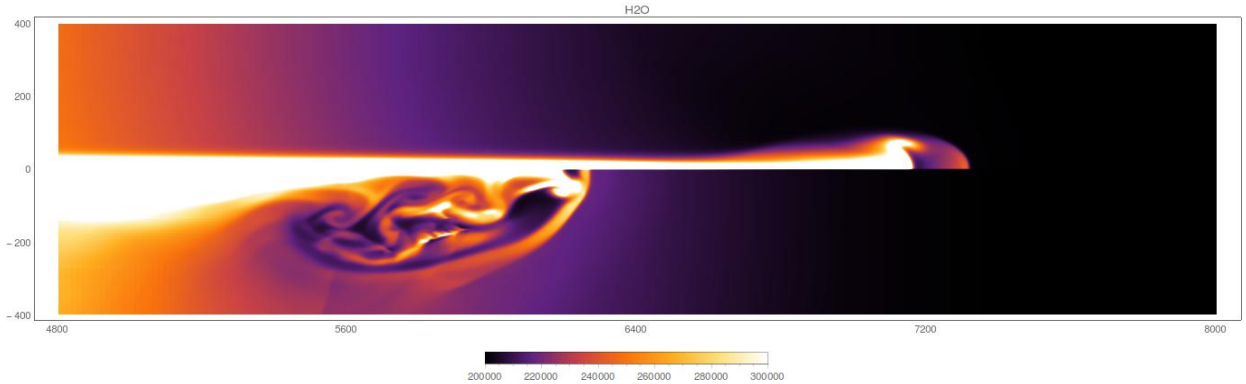


Figure : H_2O structure at 135 and 180 years. ([cm^{-3}], [AU])

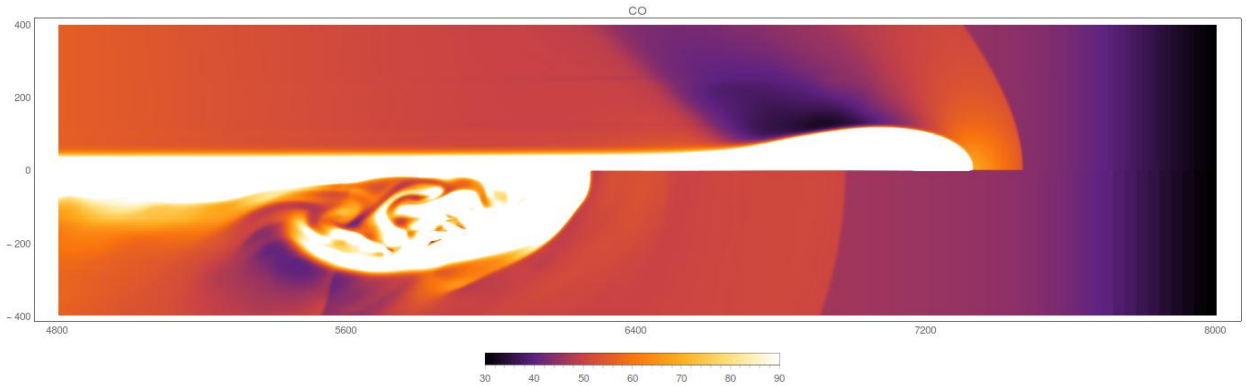


Figure : CO structure at 135 and 180 years. ([cm^{-3}], [AU])

Sumary

- **An algorithm to select reactions and create chemical networks was developed**
- **An algorithm to solve a system of ODE was programmed (KIMI)**
- KIMI **was compared to ACUCHEM, Rate 12 and tested in an atmospheric lab.**
- KIMI **was coupled into a 2D hydrodynamic code (Walicxe-2D)**

+ **Future work:**

- **Cooling**
- Propose a full formation model
- Compare simulations to Orion BN-KL and similar objets with simulations

Conclusion

Preliminary numerical simulations with the Walicxe 2D code using an adiabatic equation of state reproduce the observed morphology and kinematics of the fingers. The numerical simulations reproduce the spreading of the post-shock material orthogonal to the propagation of the bullets, the fragmentation of the leading edge of the high-velocity debris, the fingers internal structure and a density distribution for the chemical species involved. Further numerical modeling, including molecular cooling, is needed to fine-tune the model parameters to better match the relative abundances, dynamical ages and emission of the observed shocks in Orion BN-KL.

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