MODELING INTERSTELLAR SHOCKS

Sylvie CABRIT (Observatoire de Paris, LERMA)



BASIC SHOCK THEORY

- Supersonic flow meets an obstacle at Vs > sound speed
- Sudden compression → deceleration (mass conservation)
- Conversion of kinetic energy flux into
 - Thermal energy (heat)
 - Dissociation
 - Ionization
 - Magnetic energy (B compressed)
 - Internal energy → Radiation signature

If compressible obstacle (ambient cloud, previous ejecta..)

- « Forward shock » launched into the obstacle
- « Contact discontinuity » between the two shock fronts





a. Supernova Remnant: pre Sedov-Taylor Phase



c. Supernova Remnant: post Sedov-Taylor Phase



d. Stellar Wind Bubble

Outer Shock

Expanding

Stellar

Wind`

Contact Discontinuity



winds (protostars, AGB stars..) : reverse shock cools rapidly → thin shell driven by wind rampressure = « snowplow »

THIN SHELL SPEED (SNOW-PLOW)

$$\frac{d\mathcal{M}}{dt} = r^2 \rho_a v_s + r^2 \rho_w (v_w - v_s)$$
$$\frac{d\mathcal{M}v_s}{dt} = r^2 \rho_w (v_w - v_s) v_w$$

$$\Rightarrow \mathcal{M} \frac{dv_s}{dt} = \frac{d\mathcal{M}v_s}{dt} - v_s \frac{d\mathcal{M}}{dt}$$
$$= r^2 \rho_w \left((v_w - v_s)^2 - \frac{\rho_a}{\rho_w} v_s^2 \right)$$

$$\rightarrow$$
 Vs ~ $\frac{v_w}{1 + \sqrt{\rho_a/\rho_w}}$

 Shell mass increase (shocked ambient gas + shocked wind)

Shell momentum increase (from shocked wind)

 dVs/dt = 0 ←→ ram pressure equilibrium between reverse and forward shock

• Solution:
• Vs << Vw if
$$\rho_{q} >> \rho_{w}$$

SHOCK MODELING

«Forward modeling»

- Specify driving piston + ambient medium conditions
 - → compute shock front(s) structure and propagation
 - → compute emitted spectrum

« Backwards modeling » (= Inversion)

- Specify emission fluxes (observed)
 - → fit shock parameters
 - → constrain piston properties (eg. wind mass-flux, momentum flux, power, ...)
 - → constrain ambient medium properties (eg. B-field, density, ice composition,...)
 - → Constrain global **shock feedback** on ISM (turbulent support, chemistry, SF regulation...)

FORWARD MODELING

Semi-Analytical

Numerical simulations

1D, steady-state

PRO:

- Very complete non-equilibrium microphysics : ionization, chemistry, grains, ion-neutral drift...
- Fast: can compute large model grids
- Pseudo 2D = collection of 1D shocks

LIMITS:

- Ignore lateral loss of pressure in 2D
- Ignore time-dependence and instabilities

HD or MHD 1D/2D/3D

PRO:

- Exact time-dependence
- Study instabilities and turbulence
- Accurate effect of 2D curvature

LIMITS: CPU cost

- Simplified cooling and chemistry
- No large grids
- Challenging to resolve cooling length (J-shock) or treat Multi-fluid MHD (Cshock)

CONSERVATION LAWS

In the frame of shock wave

Single-fluid 1D steady-state with B // shock front

Mass conservation

 ρ V = cste

Magnetic Flux conservation

B / ρ = cste

• Momentum conservation (ram, thermal and magnetic pressure)

 $\rho V^2 + P + B^2 / 8\pi = cste$

Energy conservation

 $V [\frac{1}{2} \rho V^2 + P + u + B^2 / 4\pi] + F_{rad} = cste$

u = internal energy

 F_{rad} is radiative cooling flux

See eg. Hollenbach & McKee 1979 for oblique B case

Rankine-Hugoniot Jump conditions

set Frad = 0 (adiabatic front), case B=0

 $\rho_s = \rho_0 \frac{(\gamma + 1)\mathcal{M}^2}{(\gamma - 1)\mathcal{M}^2 + 2},$ $\rho_s \sim 4\rho_0 \text{ in the strong shock limit, } \gamma = 5/3, \, \mathcal{M} \gg 1,$

$$\frac{T_1}{T_0} = \frac{[(\gamma - 1)\mathcal{M}_0^2 + 2][2\gamma\mathcal{M}_0^2 - (\gamma - 1)]}{(\gamma + 1)2\mathcal{M}_0^2}.$$

$$T_s = \frac{2(\gamma - 1)}{(\gamma + 1)^2} \left[\frac{\mu m_u v_s^2}{k} \right],$$

~ 3000 K @ 10 km/s ~ 3 10⁵ K @100 km/s

INTEGRATED EQUATIONS

Single-fluid 1D steady-state with B // shock front In the frame of the shock wave:

- Mass conservation
- ρ V = cste
- Magnetic Flux conservation
- B / ρ = cste
- Momentum conservation (ram, thermal and magnetic pressure)

 $\rho V^2 + P + B^2 / 8\pi = cste$

Energy conservation

 $V [\frac{1}{2} \rho V^2 + P + U + B^2 / 4\pi] + F_{rad} = cste$

u = internal energy

 F_{rad} is radiative cooling flux

See eg. Hollenbach & McKee 1979 for oblique B case

- Starting from initial conditions, solve differential equations for ρ , V, P (or T), u, F_{rad} along z
- $dF_{rad} / dz = \Lambda (erg/s/cm^3) = cooling rate$
- $P = \rho kT / \mu mH$

At equilibrium, Λ , υ and μ depend only on ρ , T, elemental abundances: easy to integrate

BUT In shock cooling zone, ionization stages, molecular abundances, and internal excitation are **out of EQ** (no time to adjust)

→Also need to solve along z for each specie abundance, ionization stage, (level populations): « chemical » source terms

ENERGY CONVERSION IN SHOCKS





RADIATIVE PRECURSOR IN IONIZING SHOCKS

 UV photons emitted in shock front also propagate upstream in the preshock medium

 \rightarrow « radiative precursor »

- Vs < 40 km/s: cold neutral
- 40 < Vs < 80 km/s: warm neutral, partly dissociated
- 80 < Vs < 120 km/s : partly ionized and fully dissociated
- 120 km/s < Vs : fully ionized at IEQ

Sutherland & Dopita (2017)



Hollenbach & Mc Kee (1989)

REFERENCE 1D-SHOCK MODELS

Atomic shocks, no molecules

30 < Vs < 2000 km/s

• MAPPINGS V (Sutherland & Dopita 2017)

Public code available at https://mappings.anu.edu.au/code/

10 < Vs < 100 km/s

• Model grid in Hartigan et al. (1994, 1995)

Dissociative, with molecule reformation 30 < Vs < 120 km/s

Hollenbach & McKee 1989
 (infrared line predictions)

Non- (or weakly) dissociative Vs < 40 km/s

- No radiative precursor
- Paris-Durham shock code (Flower & Pineau des Forêts 1985 → Godard 2019)

https://ism.obspm.fr/shock.html

https://mappings.anu.edu.au/code/



An astrophysical plasma modelling code.

The MAPPINGS V Code Archive

https://mappings.anu.edu.au/code

https://bitbucket.org/RalphSutherland/mappings

Science and Programming: Ralph Sutherland, Mike Dopita, David Nicholls, Brent Groves, Luc Binette, et al

Current MAPPINGS Version V 5.1.18

v5.1.18, September 2019

Download mappings_V-5118.zip (297.8MB): Everything including stellar/agn atmospheres. SHA256 digest: 9242848db55898f6bb9359f5a739b9b52326750db5397dafc0852cf3cb6f5d22

Download M_V-5118.zip (28.7MB) : Everything except stellar/agn atmospheres. SHA256 digest: be429425e54baf0f23210b09a716ffd56583e6fa149259fa01931179e61a75a1

MAIN COOLANTS AT T > 10^4 K

Dopita+1993 cooling curve (MAPPINGS II)

Updated with CHIANTI database In MAPPINGS V



DISSOCIATIVE SHOCK WITH MOLECULE REFORMATION

- UV photons emitted in shock front reabsorbed downstream
 - «Recombination plateau » @10⁴ K (~ HII region)
 - Hydrogen lines and low-excitation ionic lines [O I], [Si II], [Fe II], etc..
- Molecule reformation plateau
 - @500 K (each H₂ molecule releases 4.48eV)
 - H₂, CO, H₂O, (+SiO, ..)



Hollenbach & Mc Kee (1989)

SHOCK SPEED DIAGNOSTICS

MAPPINGS V calculations





SPEED LIMITS IN MAGNETIZED SHOCKS

Alfven speed in neutrals

- $V_{Alfven} = B / sqrt(4 \pi \rho) = 1.8 b km/s$
- $M_A = Vs / V_{Alfven}$
- Maximum compression in postshock gas (M >> 1)

 $C = 4 M_A^2 / (1 + sqrt(1+8M_A^2))$

→ Shock compression only if $M_A > 1$

Magnetosonic speed in charged fluid

- $V_{magnet} = sqrt(C_i^2 + B^2 / 4 \pi \rho_i)$
- If V_A < Vs < V_{magnet}, magnetic compression wave propagates ahead of shock in charged fluid → « magnetic precursor »
- lons slow down by mag. pressure
- Neutrals slow down by collisions with ions → jump can disappear

J-TYPE VS C-TYPE SHOCKS

Draine (1980), Flower et al. (1985), Smith (1991), Kaufman & Neufeld (1996), Caselli et al (1997)

• V > Vmagnet (B) J (Jump)-shock = monofluid Fast dissipation by n-n collisions High Tmax ~ V²



V < Vcrit(B)

C (Continuous)-shock = **multifluid Slow dissipation by n-i collisions** Wider = Lower Tmax (H₂ cooling)



YOUNG AGE

- When age < tcool:
 - C-type magnetic « precursor » truncated at t_ion = age
 - followed by a J-type front truncated at t = age (Chièze et al. 98, Smith 98)
 - Well described by truncated steady C + J models if nH, Vs constant (Lesaffre et al. 2004)

→ Age is free parameter in the Paris-Durham model



GRAINS

- Grains dominate inertia of charged fluid (Guillet 2007)
- For gas/dust ratio ~ 100

 $V_{magnet} \sim 10 V_{Alfven} \sim 20 \text{ km/s} \text{ x b}$

Maximum speed for Cshocks

- Ion-neutral drift in C-shocks
 - → Sputtering of ice mantles
 - Releases ice species: H₂O, CH₃OH, NH₃, H₂CO...

→Erosion of grain cores Release Si → SiO (Gusdorf+2008ab)

SiO also released in J-shocks by grain-grain shattering and vaporization (Guillet 2009, 2011) Not included in public code version



EXTERNAL FUV IRRADIATION

See Godard+2019

- Extra-Free parameters: G_0 , Av_0
- Lowers H2 cooling + Increases ionization and ion-neutral coupling : narrower hotter C-shock
- \rightarrow C-shocks disappear for

 $G_0 > 0.2 \ (n_{\rm H}/{\rm cm}^{-3})^{1/2}$

and become C* (subsonic) or C-J (jump)

• Specific diagnostics: CH⁺ rotational lines, H₂ rovib (FUV pumping)





BACKWARD MODELING (INVERSION PROBLEM)

Many free parameters \rightarrow degeneracy

Ideally combine as many constraints as possible:

- Line fluxes PB: filling factor, depletion in grain+ ice → H2, CO, O
- Line ratios PB: relative depletion → single specie, or undepleted
- Shock thickness PB: spatial resolution → Hubble, JWST, ALMA
- Line profile width PB: inclination \rightarrow 2D bowshocks
- Ortho/para of H2 (if < 3)
- Ambient conditions (nH, G0, Av, zeta_CR, zeta_X) from ancillary data
- Shock Age: from speed + size



JET BOWSHOCK

- Lateral escape of shocked jet material
- Swept back by ambient gas
- Oblique shocks : Vs changes along bow surface
- Largest area at low shock speeds



UNRESOLVED 3D BOWSHOCK MODELS

Tram L.N. 2018, MNRAS

- Stitch 1D models along bow surface
- + Compute total H₂ excitation diagram
- resembles slower 1D shock ~ 10 km/s with ~ same B
- Fitting with Vs = Vbow would strongly overestimate B-field !
- Distinctive effects of density, age, bow shape, B-field strength and angle → good diagnostic potential



Tram L.N. 2018, MNRAS

FITTING H₂ IN ORION PEAK-1

• $nH = 10^6 \text{ cm}^{-3}$, age = 1000 yrs, b = 4.5

• $U_0 \ge 30 \text{ km/s}$



Line profile lifts degeneracy on bow speed ${\rm U}_{\rm 0}$ Agrees with proper motion info



Tram L.N 2018, MNRAS

RESOLVED H₂ BOWSHOCK MODELS



 Orion KL
 CISCO (H2 (v=1-0 S(1)) - Cont)

 Subaru Telescope, National Astronomical Observatory of Japan
 January 28, 1999

- 0.15'' resolution (adaptive optics)
- 3 Flux-calibrated H_2 lines (v= 1-0)



- Resolved emission thickness across bow surface
- Fit cuts by 1D shocks (Kristensen et al. 2008)
- Fit image by 3D bowshock model with projection effects (Gustafsson et al. 2010)

➔ C-shocks with

 $b = B/sqrt(nH) \sim 3-5$

agrees with unresolved bow model in Peak 1

(and polarization data)





ORTHO/PARA RATIO OF

- Spectrally resolved observations in HH7 (EXES/SOFIA)
- Velocity shift between ortho and para H2 lines → large OPR variation
- only explained with C-shock model (10⁴ cm⁻³, 20 km/s, 130microG)
- (Neufeld+2018)



OTHER MOLECULES

- Flower & Pineau des Forêts 2010: CO and H₂O in C and J shocks
- Flower et al. 2010: Methanol in C-shocks
- Flower & Pineau des Forêts 2012: NH₃ emission in Cshocks, Effect of age, revised methanol and ammonia ice abundances
- Pineau des Forêts et al. 2013 : OH emission as diagnostic of C vs. J shocks
- Flower et al. 2015 : detailed code description and updated atomic + molecular line predictions using LVG escape formalism

- NB: NH3 in C-shocks depends on assumed initial ice abundance (illknown)
- NB2: absolute fluxes depend on « filling-factor » → look at relative line fluxes (excitation diagrams)

C VS J DIAGNOSTICS





EXAMPLE: IRAS4A

• Herschel PACS data

Flower & Pineau des Forêts 2013



DOUBLE SHOCK STRUCTURE

« BOLOMETRIC METHOD »

% of kinetic energy flux $\frac{1}{2} \rho V_s^3$ radiated by shock tracers:

 H₂ main coolant in non-dissociative shocks (25%-80%): useful « bolometric » tool at Vs < 30 km/s

 CO % and H₂O % depend too strongly on (nH,Vs) (but improve total % if added to H₂)

 O and H lines → dissociative Jshocks

	$n_{\rm H}$ (cm ⁻³)	$\frac{v_s}{(\text{km s}^{-1})}$	H ₂ O (per cent)	H ₂ (per cent)	CO (per cent)	O (per cent)	Ly α (per cent)	Total (per cent)
	2×10^{4}	10	1.9	34.2	17.0	0.7	_	53.8
	2×10^4	20	11.0	57.0	4.9	0.01	_	72.9
	2×10^4	30	6.8	72.7	2.1	_	_	81.6
C-type	2×10^4	40	4.3	80.6	1.1	_	_	86.1
	2×10^5	10	4.9	26.2	19.6	0.1	_	50.8
	2×10^5	20	17.1	48.8	3.9	_	_	69.8
	2×10^5	30	9.6	69.3	1.4	_	_	80.4
	2×10^5	40	5.9	79.5	0.7	_	_	86.1
	2×10^4	10	32	75.5	6.8	_		85.5
J-type	$\frac{2}{2} \times 10^{4}$	20	15.0	72.5	9.0	0.01	_	96.6
0 . 7 0 0	2×10^4	30	18.7	3.3	0.8	6.6	41.1	80.4
	2×10^5	10	5.7	64.5	3.6	_	_	73.8
	2×10^5	20	50.7	15.1	5.8	1.8	_	73.3
	2×10^{5}	30	23.3	3.0	0.1	2.6	48.2	77.3

H₂ BOLOMETRIC METHOD APPLIED

Maret et al. 2009

 Spitzer: H₂ pure rotational lines from outflows in NGC1333 (green in image)

C-shocks at Vs ~ 20-30 km/s

- L(H2) → KE flux in shock = Lmech
 - → Momentum injection rate :

 $P_s = 2 Lmech / Vs$

= $2-5 \ 10^{-5} \text{ MO km/s/yr}$ per flow

• After 2x10⁵ yr, each flow imparts 1 km/s turbulence in 5M⊙

20 flows: 100 Mo= 30% of cloud mass



« BOLOMETRIC METHOD » FOR DISSOCIATIVE SHOCKS

 8×10^{-14}

1.E+00

- [O I] 63mic flux is (roughly) proportional to mass-flux into shock (Hollenbach 1985)
- Same for [Fe II]26mic and [Si II]35mic

$$\dot{M}_{w} = 8.1 \times 10^{-5} L([\text{O I}] \ 63.2 \ \mu\text{m}) \frac{M_{\odot} \ \text{year}^{-1}}{L_{\odot}}$$
$$= 9.8 \times 10^{-4} L([\text{Si II}] \ 34.8 \ \mu\text{m}) \frac{M_{\odot} \ \text{year}^{-1}}{L_{\odot}}$$
$$= 1.4 \times 10^{-3} L([\text{Fe II}] \ 26.0 \ \mu\text{m}) \frac{M_{\odot} \ \text{year}^{-1}}{L_{\odot}}.$$



Watson+2016

LIMITATIONS OF « BO

- Several shock fronts contribute to [O I] not just the final terminal shock
 - Overestimate mass-flux in jet/wind
- Need spectrally (SOFIA-GREAT, EXES) and spatially (JWST, ALMA, NOEMA) resolved observations of shocks to separate components





CONCLUSIONS

- Interstellar shock waves are complex systems to model, but very detailed public 1D models exist for different shock regimes
- Backward inversion is difficult exercice
 - Many free parameters: beware of degeneracies, combine constraints !
 - Several key atomic coolants (Fe+, S, Si+) may have grain depletion
 - When non-dissociative: Output radiation depends on preshock chemical conditions (ice mantles + ambient G0 and zeta): necessary to use self-consistent preshock before running models
 - May have several shock fronts in beam (reverse J + forward C): favor high angular resolution and spectral resolution: JWST, SOFIA and ALMA
- Fast progress in 2D/3D simulations including NEQ chemistry: new tool