Heating of the Interstellar gas
theory and implementation

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Before to start

Heating in KROME

- UNITS: erg cm^{-3} s^{-1}
- OPTION: -heating

```
$ ./krome -n network.ntw -heating=?

******************************
    WELCOME TO KROME
******************************

Available heatings are: COMPRESS, PHOTO,
   CHEM, CR, PHOTOAV, PHOTODUST,
   PHOTODUSTNET, XRAY, VISCOUS
```

Introduction

There are different ways to heat the gas in the ISM, i.e. to transfer energy into the gaseous medium

- via photons/electrons
- via chemical reactions
- via dust grains
- via dynamical processes

Main processes:

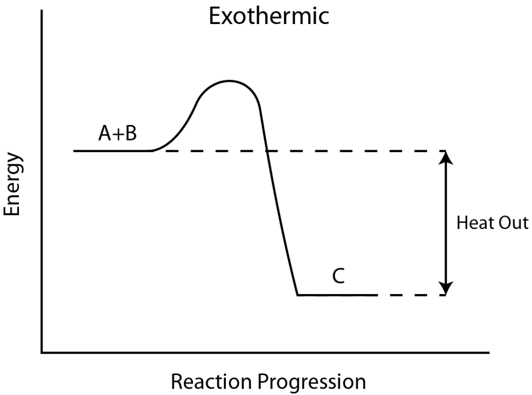
- elastic collisions
- collisional de-excitations

(1) Chemical heating

Chemical heating

formation of molecules

$$A + B \rightarrow C + \Delta H$$



Chemical heating (cont'd)

formation of molecules

the energy can be released as/in:

- translation energy of the newly formed molecule
- rotational/vibrational excitations
- if on grains → heat the grains

heating occurs via

- collisional de-excitations
- simple collisions

Chemical heating (cont'd)

formation of molecules

MAIN UNCERTAINTY

distribution between the different forms of energy

Chemical heating (cont'd)

formation of molecules

$$A + B \xrightarrow{k_i} C + \Delta \mathrm{H}$$

$$\boxed{\Gamma_{chem} = k_i n_A n_B \epsilon_i \Delta \mathrm{H}}$$

$$\begin{aligned}
\mathrm{H^- + H} &\rightarrow \mathrm{H_2} + \mathrm{e^-} + 3.53\ \mathrm{eV} \\
\mathrm{H_2^+ + H} &\rightarrow \mathrm{H_2} + \mathrm{H^+} + 1.83\ \mathrm{eV} \\
\mathrm{H + H + H} &\rightarrow \mathrm{H_2} + \mathrm{H} + 4.48\ \mathrm{eV} \\
\mathrm{H_2 + H + H} &\rightarrow \mathrm{H_2} + \mathrm{H_2} + 4.48\ \mathrm{eV} \\
\mathrm{H + H + GR} &\rightarrow \mathrm{H_2} + \mathrm{GR} + 4.48\ \mathrm{eV}
\end{aligned}$$

$$\boxed{\epsilon_i = \left(1 + \frac{n_{cr}}{n}\right)^{-1}}$$

Chemical heating (cont'd)

efficiency

$$\boxed{\epsilon_i = \left(1 + \frac{n_{cr}}{n}\right)^{-1}}$$

$$n_{cr} = \frac{A_{ul}}{\gamma_{ul}}$$

- critical density

- if $n >> n_{cr} \rightarrow \epsilon_i = 1$ & $\Delta \mathrm{H} \rightarrow$ heats the gas
- if $n << n_{cr} \rightarrow \epsilon_i \sim 0$ & $\Delta \mathrm{H} \rightarrow$ radiates away

Chemical heating (cont'd)

efficiency

$$\boxed{\epsilon_i = \left(1 + \frac{n_{cr}}{n}\right)^{-1}}$$

$$n_{cr} = \frac{A_{ul}}{\gamma_{ul}}$$

- critical density
- ratio between Einstein coefficient and the collisional de-excitation rate

- if $n >> n_{cr} \rightarrow \epsilon_i = 1$ & $\Delta\mathrm{H} \rightarrow$ heats the gas
- if $n << n_{cr} \rightarrow \epsilon_i \sim 0$ & $\Delta\mathrm{H} \rightarrow$ radiates away

Chemical heating (cont'd)

H_2 efficiency

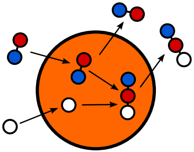
Hollenbach& McKee 1979:

$$\begin{aligned}\gamma_{20}^{\mathrm{H}} &= 1.6\times10^{-12}\,T^{1/2}\exp[-(1000/T)]\ \mathrm{cm}^3\ \mathrm{s}^{-1}\\ \gamma_{10}^{H_2} &= 1.4\times10^{-12}\,T^{1/2}\exp\{-[12000/(T+1200)]\}\ \mathrm{cm}^3\ \mathrm{s}^{-1}\\ A &= 10^{-6}\ \mathrm{s}^{-1}\end{aligned}$$

$$\boxed{n_{cr}=\frac{10^6\,T^{1/2}}{1.6\exp[-(1000/T)]+1.4\exp\{-[12000/(T+1200)]\}}}$$

Chemical heating (cont'd)

H_2 formation on dust



$$\boxed{\mathrm{H} + \mathrm{H} + \mathrm{GR} \rightarrow \mathrm{H}_2 + \mathrm{GR} + 4.48\ \mathrm{eV}}$$

- most relevant process
- energy distributed as following
  - 0.2 eV as kinetic energy
  - 4.2 eV in roto-vibrational state of H_2
  - heating of grain negligible

$$\boxed{\Gamma^d_{\mathrm{H}_2} = R_f(0.2 + 4.2\epsilon)n_{tot}n_{\mathrm{H}}}$$

WARNING: different rates available

Chemical heating (cont'd)

H_2 formation on dust

$$\boxed{\Gamma^{d}_{\mathrm{H_2}} = R_f(0.2 + 4.2\epsilon)n_{tot}n_{\mathrm{H}}}$$

$$
\begin{aligned}
{}^{1}R_f &= 3\times10^{-17}\\
{}^{2}R_f &= 3\times10^{-17}\frac{T_2^{0.5}f_a}{1+0.4(T_2+T_{d_2})^{0.5}+0.2T_2+0.09T}\\
{}^{3}R_d &= 0.5v_g\pi a^2\varepsilon_{\mathrm{H_2}}S(T,T_d)n_{\mathrm{H}}n_d
\end{aligned}
$$

Note $R_d(\mathrm{H_2})$ is the overall rate of H_2 formation in terms of cm^{-3} s^{-1}, to compare

$$\boxed{\Gamma^{d}_{\mathrm{H_2}} = R_d(0.2 + 4.2\epsilon)}$$

$$R_d(\mathrm{H_2}) = R_f n n_{\mathrm{H}} \quad (1)$$

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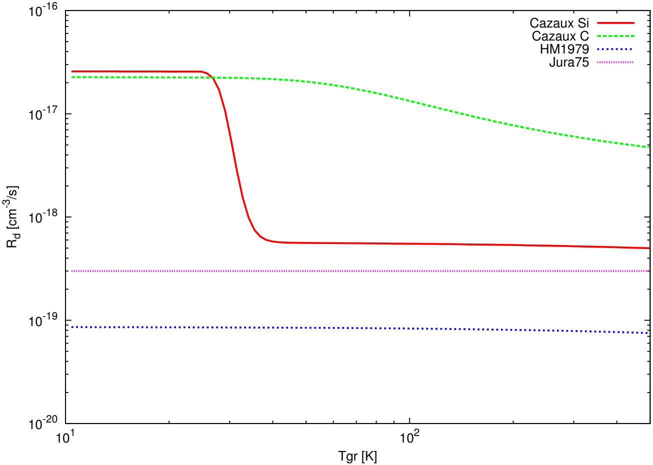
[1] Jura 1975

[2] Hollenbach& McKee 1979

[3] Cazaux & Tielens 2004

Chemical heating (cont'd)

H_2 formation on dust



$$n = 0.1\ \mathrm{cm}^{-3},\ n_d\sigma \sim 10^{-21}\ \mathrm{cm}^2,\ T_{gas} = 300\ \mathrm{K}$$

Chemical heating in KROME

in KROME_HEATING.F90

```
$ ./krome -n network.ntw -heating=CHEM

*****************************************
function heatingChem(n, Tgas, k, nH2dust)

...
...

!H + H + H -> H2 + H (heating)
  HChem = k(25) *
     (4.48d0*h2heatfac*n(idx_H)*n(idx_H)*n(idx_H)

 heatingChem = HChem * eV_to_erg !erg/cm3/s

end function heatingChem
```

Chemical heating in KROME

Things to know:

- chemical cooling is also included in KROME_HEATING.F90 by construction
- mainly H_2 formation heating
- KROME option CHEM
- only active if you have that given reaction in your network

Chemical heating

Further reading:

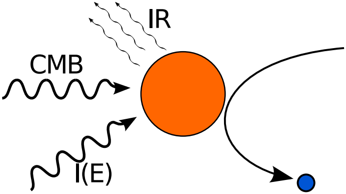
- J. Lequeux "The Interstellar Medium" 2003
- A. Tielens "The physics and chemistry of the Interstellar Medium" 2005
- Dalgarno & Oppenheimer 1974
- Hollenbach & McKee 1979
- Burke & Hollenbach 1983
- Cazaux & Tielens 2004

(2) Grain-gas thermal exchange

Grain-gas thermal exchange

basics

- the grain size ($\Gamma \propto \pi a^2$)
- dust and gas temperature
- gas velocity $v_g = \sqrt{\dfrac{8 k_b T_g}{\pi m_{\rm H}}}$



$$\Gamma_{\rm em} = \Lambda_{\rm g\to d} + \Gamma_{\rm CMB} + \Gamma_{\rm abs}$$

$$\boxed{\Lambda_{g\to d}(a, T_d) = 2\pi a^2 n_g n_d v_g k_b (T_g - T_d)\alpha} \quad T_g > T_d \rightarrow \text{cooling}$$

$$\boxed{\Gamma_{g\to d}(a, T_d) = 2\pi a^2 n_g n_d v_g k_b (T_d - T_g)\alpha} \quad T_d > T_g \rightarrow \text{heating}$$

Grain-gas thermal exchange

accomodation coefficient

every collision gives to the gas a mean energy:

$$E = 2\alpha k(T_d - T_g) \longrightarrow \boxed{\alpha = \frac{T_2 - T_g}{T_d - T_g}}$$

how efficiently energy is shared between the dust and the gas

MAIN UNCERTAINTY

EVALUATE THE ACCOMODATION COEFFICIENT

Grain-gas thermal exchange

accomodation coefficient

it depends on

- nature of dust grains
- nature of colliders
- T_g and T_d

In literature

- $\alpha = 0.3$ fully molecular gas[4]
- $\alpha = 1$ common

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[4] Burke & Hollenbach 1985

Grain-gas thermal exchange

approximated formulae

Expressions in literature for $\Gamma_{g\to d}$ typically written:

$$\boxed{\Gamma_{g\to d} = C_{g\to d} T_g^{1/2} (T_d - T_g) n^2}$$

$C_{g\to d}$ in units of erg cm^{-3} s^{-1} K$^{3/2}$

$$^{5}C_{g\to d} = 3.8\times 10^{-33}\left[1 - 0.8\exp\left(\frac{-75\ \mathrm{K}}{T_g}\right)\left(\frac{10^{-6}\mathrm{cm}}{a_{min}}\right)^{1/2}\right]$$

$$^{6}C_{g\to d} = 3.5\times 10^{-34}$$

$$^{7}C_{g\to d} = 6.3\times 10^{-34}$$

- intended for use in H_2-dominated regions
- assumptions made on $n_d\sigma_d$

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[5] Hollenbach& McKee 1989

[6] Tielens & Hollenbach 1985

[7] Goldsmith 2001

Grain-gas thermal exchange

in KROME

$$\boxed{\Gamma_{g\rightarrow d}(a, T_d) = 2\pi a^2 n_g n_d v_g k_b (T_d - T_g)\alpha}$$

You have to enable the dust machinery

```
$ ./krome -n network.ntw -dust=1,C
   -cooling=DUST
```

- based on the grain-size distribution and grain properties
- only assumption on the free parameter α
- re-scaled by the metallicity (dust-to-gas ratio)

See Tommaso's talk on Thursday!

Grain-gas thermal exchange

when is important

- at high densities (high # of collisions)
- SNa remnants grain heating is dominant (both T_g and $n >>$)
- HII regions: $\Gamma_{g\rightarrow d} << \Gamma_{ph}$
- negligible in PDR and WIM

Gas-grain thermal exchange

references

Further reading:

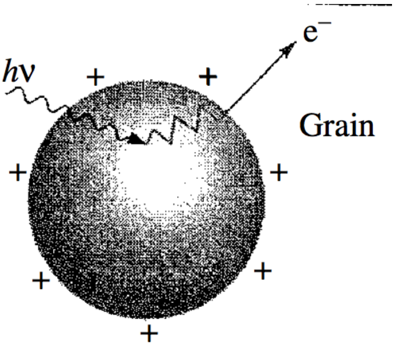
- J. Dyson, D. A. Williams "The physics of the Interstellar Medium" 1997
- J. Lequeux "The Interstellar Medium" 2003
- A. Tielens "The physics and chemistry of the Interstellar Medium" 2005
- Burke & Hollenbach 1983
- Tielens & Hollenbach 1985
- Hollenbach & McKee 1989
- Goldsmith 2001

(3) Photoelectric heating

Photoelectric heating

basics

- most important heating process in the cold neutral ISM
- UV radiation from hot stars remove e^- from interstellar dust grains.



Photoelectric heating (cont'd)

basics

$$\boxed{\mathcal{H}(a,q) = 4\pi \int_{\nu_q}^{\nu_H} \frac{J_\nu}{h\nu} \sigma_{abs}(a,\nu) Y_{ion}(a, IP_q) g(a, IP_q) d\nu}$$

$\boxed{J_\nu}$ → radiation intensity in erg cm^{-2} s^{-1} sr^{-1}

$\boxed{h\nu_q = IP_q = W + \phi}$ → ionization potential

$\boxed{\sigma_{abs} = Q_{abs}\pi a^2}$ → absorption cross-section

$\boxed{Y_{ion}}$ → # of photoelectrons ejected per absorbed photon

$\boxed{g}$ → partition function of the kinetic energy of the photoelectrons

$\boxed{h\nu_H}$ → Hydrogen ionization potential

Photoelectric heating (cont'd)

basics

For a given grain size distribution n(a) da:

$$\boxed{\Gamma_{pe} = \int_{a_{min}}^{a_{max}} \sum_q H(a,q) f(a,q) n(a) da}$$

Reaction to be taken into account

$$\mathrm{GR}^{+(n)} + \gamma \rightarrow \mathrm{GR}^{+(n+1)} + \mathrm{e}^- \quad (2)$$

$$\mathrm{GR}^{+(n)} + \mathrm{e}^- \rightarrow \mathrm{GR}^{+(n-1)} \quad (3)$$

$$\mathrm{GR}^{+(n)} + \mathrm{A}^+ \rightarrow \mathrm{GR}^{+(n+1)} + \mathrm{A} \quad (4)$$

$$\boxed{\Gamma_{pe}^{net} = \int_{a_{min}}^{a_{max}} \sum_q [H(a,q) - C(a,q)] f(a,q) n(a) da}$$

Photoelectric heating (cont'd)

MAIN PROBLEM

EVALUATE THE CHARGE OF THE GRAINS!

charge equilibrium problem!

$$\boxed{f(q)[J_{pe}(q)+J_{ion}(q)] = f(q+1)J_e(q+1)}$$

- photoelectron emission
- accretion rate of ions
- accretion rate of electrons

Photoelectric heating (cont'd)

parametrization see Bakes & Tielens 1994

$$\boxed{\gamma = \left(\frac{G_0 T_{gas}^{1/2}}{n_e}\right)} \rightarrow \text{charging parameter}^{8}$$

$$\boxed{\epsilon = \frac{4.87 \times 10^{-2}}{1 + 4 \times 10^{-3}\gamma^{0.73}} + \frac{3.65 \times 10^{-2}\left(T/10^4\right)^{0.7}}{1 + 2 \times 10^{-4}\gamma}}$$

$$\Gamma_{pe}^{net} = \Gamma_{pe} - \Lambda_{rec}$$

$$\Gamma_{pe} = 1.3 \times 10^{-24}\epsilon G_0 n_H$$

$$\Lambda_{rec} = 4.65 \times 10^{-30} T_{gas}^{0.94}\gamma^{\beta} n_e n_H \quad with\ \beta = 0.735 T^{-0.068}$$

assumption: grains absorb a UV energy of 10^{-24} erg s^{-1} per hydrogen atom (at $Z = Z_{\odot}$).

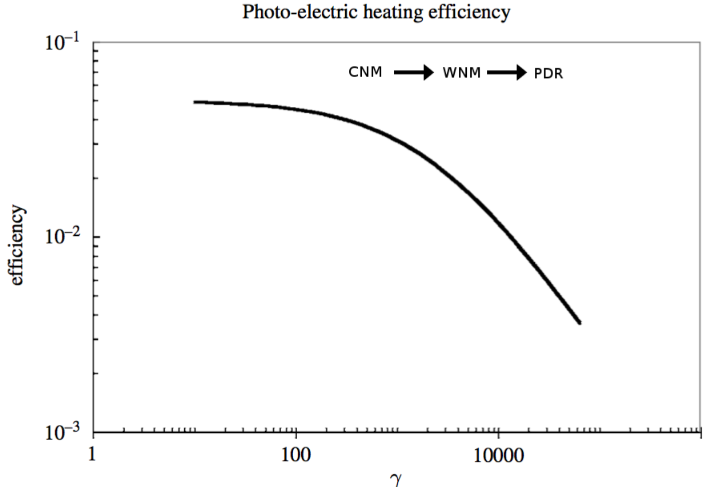
---

[8] $G_0 \rightarrow$ Habing flux, i.e. $u(6 - 13.6eV)/5 \times 10^{-14}$ erg cm^{-3}

Photoelectric heating (cont'd)

efficiency ϵ

$$\boxed{\gamma = \left(\frac{G_0 T_{gas}^{1/2}}{n_e}\right)}$$



Photoelectric heating (cont'd)

to keep in mind

Three main parameters influence the photoelectric heating rate

i) the strength of the radiation J_ν
ii) the size distribution of the grains
iii) the charge of the grains

Assumptions and summary

- PE heating mostly acts on small grains ($a \leq 100$ Å)
- PE heating most important process in CNM
- HII region heating dominated by photoheating
- in the model only C-like grains considered
- recombination negligible in CNM ($G_0 \sim 1$)

Photoelectric heating in KROME

```
$ ./krome -n network.ntw -heating=?

******************************
     WELCOME TO KROME
******************************

ERROR: Heating "?" is unknown!
Available heatings are: COMPRESS, PHOTO,
    CHEM, DH, CR, PHOTOAV, PHOTODUST,
    PHOTODUSTNET, XRAY, VISCOUS

$ ./krome -heating=PHOTODUST
$ ./krome -heating=PHOTODUSTNET
```

Photoelectric heating in KROME

PHOTODUST

- assume a local interstellar Habing flux $G_0 = 1.69$
- do not consider the recombination cooling
- rescaled by the metallicity $Z/Z_\odot$

PHOTODUSTNET

- assumes a generic flux J_ν
- does include the recombination cooling
- rescaled by the metallicity $Z/Z_\odot$

Photoelectric heating

references

Further reading:

- J. Lequeux "The Interstellar Medium" 2003
- A. Tielens "The physics and chemistry of the Interstellar
- Draine & Sutin 1987
- Bakes & Tielens 1994 Medium" 2005

Heating

(4) UV heating

Heating induced by radiation (1)

UV photons

$$\begin{aligned} \mathrm{A}^{+\mathrm{n}} &+ h\nu \rightarrow \mathrm{A}^{+(\mathrm{n}+1)} + \mathrm{e}^- \\ \mathrm{AB} &+ h\nu \rightarrow \mathrm{AB}^+ + \mathrm{e}^- \\ \mathrm{AB} &+ h\nu \rightarrow \mathrm{A} + \mathrm{B} \end{aligned}$$

The photodissociation and photoionization[9] induced by FUV radiation generate an excess of energy which can go into heating $(h\nu - E_0)$.

Photoheating is mainly caused by

- atoms photoionization in HII regions ($h\nu > 13.6$ eV)
- photo-ionization of large molecules and small dust grains in HI regions ($h\nu < 13.6$ eV)
- molecules photodissociation in molecular regions

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[9] Wing-Fai Thi's talk

Heating induced by radiation (1)

UV photons

$$H_{ph}[\mathrm{erg\ s^{-1}}] = \frac{4\pi}{h}\int_{E_0}^{\infty}\frac{J(E)\sigma(E)}{E}(E-E_0)\eta(E)e^{-\tau}dE$$

$\eta(E)$ is an efficiency factor that determines the amount of energy released into the gas.

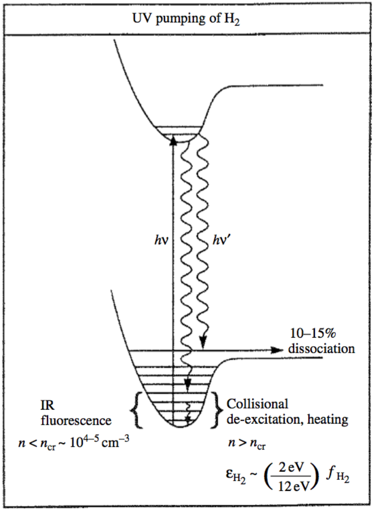
The effective photoheating is

$$\boxed{\Gamma_{ph} = H_{ph}n_X \ \ \mathrm{erg\ s^{-1}cm^{-3}}.}$$

Heating induced by radiation (1)

H_2 UV pumping

$$\boxed{H_2 + h\nu \rightarrow H_2^* \rightarrow H + H}$$



Heating induced by radiation (1)

H_2 UV pumping

- Lyman-Werner bands (11.2-13.51 eV)
- 0.4 eV $\rightarrow 6.4\times\,10^{-13}$ erg per dissociation (kinetic energy)
- 2.2 eV $\rightarrow 3.5\times\,10^{-12}$ erg due to vibrational de-excitation

$$\boxed{\Gamma^{UV}_{pd_1} = 9R_{pd}(\mathrm{H}_2)\{3.5\times10^{-12}\,[1+n_{cr}/n]^{-1}\}n_{\mathrm{H}_2}}$$

$$\boxed{\Gamma^{UV}_{pd_2} = 6.4\times10^{-13}R_{pd}(\mathrm{H}_2)\eta n_{\mathrm{H}_2}}$$

$$\boxed{\Gamma^{tot}_{pd} = \Gamma^{UV}_{pd_1} + \Gamma^{UV}_{pd_2}} \rightarrow \text{total heating}$$

- η = 0.1 (only 10% of the molecules dissociate)

Heating induced by radiation (1)

in KROME

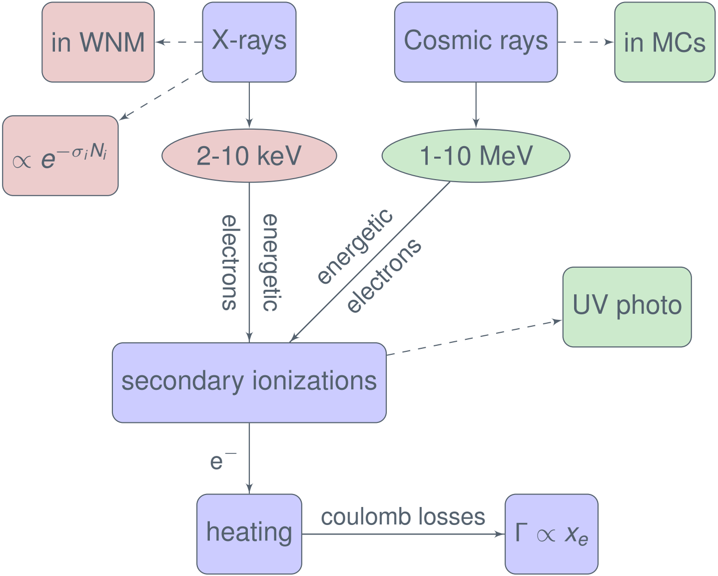
two different options:

- -heating = PHOTO
  - ionization of atoms and molecules
  - direct photodissociations
  - whatever with a cross-section
  - no H_2 UV pumping included (till now)
  - ν-dependent photochemistry needed
- -heating = PHOTOAV
  - A_v approximation
  - mainly for local ISM/MC applications
  - assume a radiation of $G_0 = 1.7$
  - includes H_2 UV pumping
  - no photochemistry needed (only $A_v(N_i)$ evaluation)

(5) X-rays/cosmic-rays heating

Heating induced by radiation (2)

a schematic overview



in WNM

X-rays

Cosmic rays

in MCs

$\propto e^{-\sigma_i N_i}$

2-10 keV

1-10 MeV

energetic electrons

energetic electrons

UV photo

secondary ionizations

e^-

heating

coulomb losses

$\Gamma \propto x_e$

Heating induced by radiation (2)

X-rays photons

$$H_x = \frac{4\pi}{h} \int_{E_0}^{\infty} \frac{J_x(E)\sigma(E)}{E} E_h(E, x_e)\, e^{-\tau} dE$$

- fraction of primary e^- energy which goes into heating

$$\boxed{\Gamma_x^i = H_x^i n_i}$$

For hydrogen and helium:

$$^{10}E_h(E, x_e) = (E - E_0)0.9971[1 - (1 - x_e)^{0.2663}]^{1.3163}$$

---

[10] Shull & van Steenberg 1985

Heating induced by cosmic rays

see Daniele Galli's talk for details

- every CR process releases $\sim$ 35 eV of energy
  - heating
  - secondary ionizations

$$\boxed{\Gamma^i_{CR} = Q k_i^{cr} n_i} \rightarrow \boxed{\Gamma^i_{CR} = Q \alpha_i \xi_{cr} n_i}$$

- great uncertainty in the fraction of heating
- it varies depending on the environment (if neutral or ionized)
  - $Q = 7.7$ eV at 2 MeV → Glassgold & Langer 1973
  - $Q = 6.6$ eV at 2 MeV → Cravens & Dalgarno 1978
  - $Q = 6 - 35$ eV → Shull & van Steenberg 1985
  - $Q = 7.0$ eV → Stahler & Palla 2004
  - $Q = 20$ eV → Goldsmith 2001
  - $Q = 13$ eV → Glassgold, Galli, & Padovani 2012
- uncertainty also on ξ_{cr}
  - $\xi_{cr} = 1 - 2 \times 10^{-17}$ s^{-1} → a kind of standard

Heating induced by cosmic rays

NOTE: the uncertainty introduced by using an averaged Q is typically much smaller than the current uncertainty in the ξ_{cr} in the considered region!

Heating induced by radiation (2)

X-rays in KROME

- -heating = `XRAY`
- check react_xrays to see how to use the X-rays tokens
- rates and heating (H and He) pre-integrated (tables)
- [11] $J_x(E) = 10^{-21} J_{21} (E/E_0)^{-1.5} \rightarrow E_0 = 1$ keV

```
#Photoionization of H, He by Xrays,
   Shull+1985, Inayoshi+2012
@XRAY_start
@format:idx,R,P,P,Tmin,Tmax,rate
24,H,H+,E,NONE,NONE,auto
25,He,He+,E,NONE,NONE,auto
@XRAY_stop
```

---

[11] Glover & Brand 2003

Heating induced by cosmic rays

in KROME

Current implementation of CR in KROME:

- CR ionization rates from OSU database
- $Q = 20$ eV
- option: -heating = CR

In the network file use the following tokens

```
@CR_start
257,H,H+,E,4.6d-1*user_crFlux
258,He,He+,E,5.d-1*user_crFlux
259,O,O+,E,2.8d0*user_crFlux
@CR_stop
```

Heating induced by radiation (2)

references

Further reading:

- Shull & van Steenberg 1985
- Wolfire et al. 1995
- Ricotti, Gnedin & Shull 2002
- Ricotti & Ostriker 2004
- Meijerink & Spaans 2005
- Valdés & Ferrara 2008
- Furlanetto & Stoever 2010

Dynamical processes

macroscopic heating

- heating at macroscopic scales
- comes from hydro → not in KROME

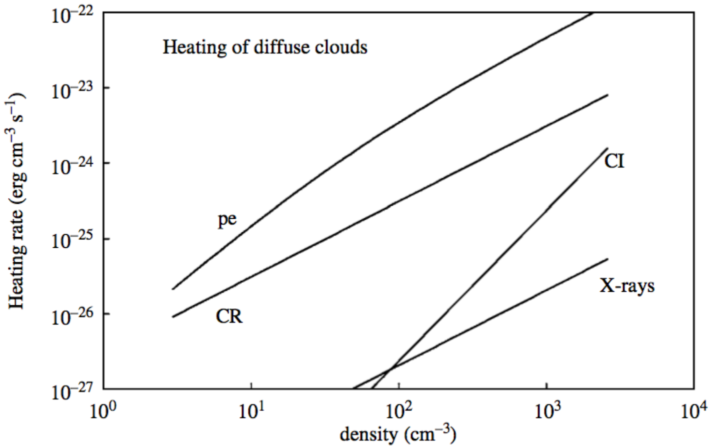
Examples:

- compressional → e.g. during gravitational collapse
- shocks/turbulence
- mechanical → stellar winds/SNe explosion
- viscous heating (e.g. ambipolar diffusion)

Overview

diffuse clouds

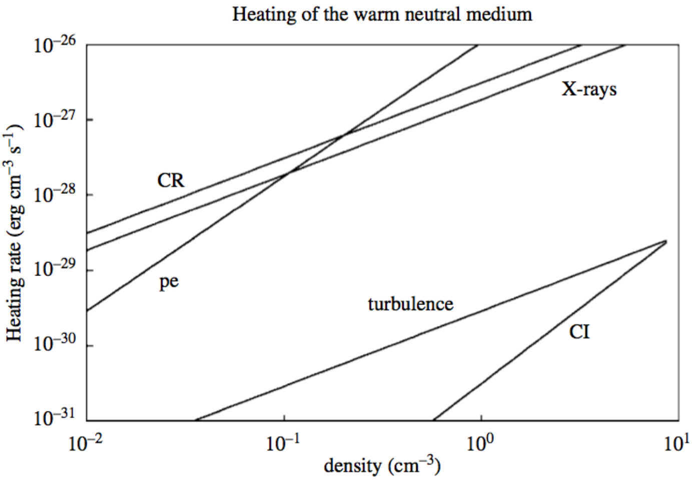
$T = 100$ K, $G_0 = 1$, $x_e = 1.2 \times 10^{-4}$



Overview

warm neutral medium

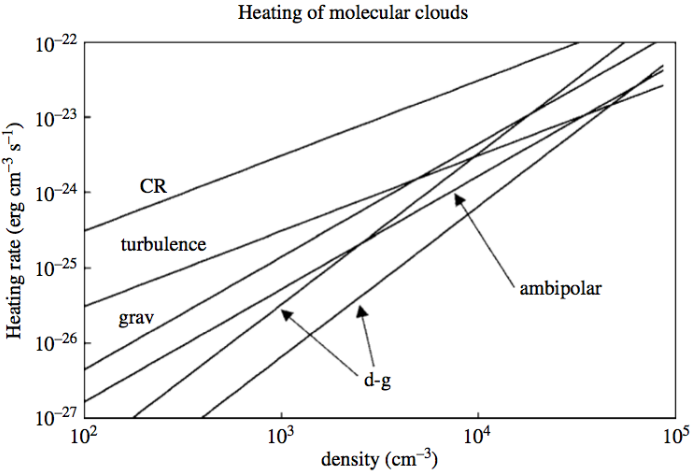
$T = 8000$ K, $G_0 = 1$, $x_e = 3 \times 10^{-3}$, $\xi_{cr} = 2 \times 10^{-16}$ s^{-1}



Overview

molecular clouds

$T = 10$ K, no FUV/X-rays rad, $x_e = 1 \times 10^{-7}$



Summary

- grain-gas → `-cooling=DUST`
  - need to enable the dust machinery
- photoelectric
  - `-heating=PHOTODUST`
  - `-heating=PHOTODUSTNET`
- chemical → `-heating=CHEM`
  - mostly H_2 processes
- photoheating → `-heating=PHOTO`
  - need to enable the photochemistry
- X-rays → `-heating=XRAY`
  - tabulated H/He rates/heating
- cosmic rays → `-heating=CR`
  - assuming 20 eV per ionization

`www.kromepackage.org`

Thank you for your attention!