PDR-Model Characteristics[1]

Contents

[1] written by M.Röllig, updated 6.Nov.2003

Mark all matching characteristics of Your PDR-Model with a X in the corresponding brackets (like (X)). Please try to give full references as far as possible. Additional remarks, which do not fit to any of the given questions can be added at the end of the questionnaire. Please contact M.Röllig (roellig@ph1.uni-koeln.de) for comments or additions.

1 Model Identification

Name of the Model . . . .

List of Authors . . . .

Institute . . . .

Contact Email . . . .

Model has been presented/discussed in (Ref.): . . . .

. . . .

. . . .

Additional Info . . . .

. . . .

. . . .

. . . .

2 Geometry

( ) spherical

( ) plane-parallel (semi-infinite)

( ) plane-parallel (finite)

( ) ensemble of clouds (Ref.: . . . .)

( ) other (Ref.: . . . .)

Density

- **( )** homogeneous
- **( )** density gradient (Eq.: . . . .)
- **( )** velocity field (Eq.: . . . .)
- **( )** time dependant geometry (. . . .)

3 Radiation Field

( ) isotropic[2] (Ref.: . . . .)

( ) uni-directional (Ref.: . . . .)

( ) other (Ref.: . . . .)

3.1 Radiation sources

( ) external source

- ( ) Habing field
- ( ) Draine field
- ( ) Other (Ref.: . . . .)
- ( ) detailed spectral energy distribution (Ref.: . . . .)

( ) internal source

- ( ) Habing field
- ( ) Draine field
- ( ) Other (Ref.: . . . .)
- ( ) detailed spectral energy distribution (Ref.: . . . .)

4 Chemistry

( ) time dependant solution(Ref.: . . . .)

( ) stationary solution(Ref.: . . . .)

Underlying Database

- ( ) UMIST95
- ( ) UMIST99
- ( ) NSM
- ( ) other (Ref.: . . . .)

extension of database:

Ref.: . . . .
Ref.: . . . .
Ref.: . . . .

[2] The important difference between isotropic vs. unidirectional or collimated radiation is the resulting local mean intensity. If one just accounts for a uni-directional radiation field the mean intensity $\bar{J}$ just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain I_ν.

( ) fixed number of included species (number: ....)

( ) variable number of included species (.........-.........)

( ) PAH's included (Ref.: . . . .)

( ) depletion on grains/ice included (Ref.: . . . .)

( ) formation of H_2 on grains (Ref./Eq.: . . . .)

( ) formation of other molecules on grains (Ref./Eq.: . . . .)

( ) desorption mechanisms included

- ( ) photoevaporation
- ( ) CR spot heating
- ( ) grain-grain collisions
- ( ) grain sputtering

( ) metallicity effects included

- ( ) scaling law[3] for elemental abundances (Eq./Ref.: . . . .)
- ( ) scaling law[3] for dust abundance (Eq./Ref.: . . . .)
- ( ) scaling law[3] for PAH abundance (Eq./Ref.: . . . .)
- ( ) metallicity dependant heating rates (Ref.: . . . .)
- ( ) metallicity dependant cooling rates (Ref.: . . . .)

( ) isotopomers included

- ( ) D
- ( ) ^{13}C
- ( ) ^{17}O
- ( ) ^{18}O
- ( ) . . . .
- ( ) . . . .

( ) other . . . .

( ) other . . . .

[3] functional interrelation e.g. $X(C)=Z^{\alpha}\times X(C)$

5 Thermal Balance

( ) fixed temperature law (Eq.: . . . .)

( ) temperature determined from energy balance

Cooling Functions

- **( )** gas-grain cooling (Ref.: . . . .)
- **( )** radiative line cooling (details in section 6.2)
- **( )** . . . .
- **( )** . . . .

Heating Functions

- **( )** H_2^* vibrational deexcitation
  - **( )** single line approximation(Ref.: . . . .)
  - **( )** only ν-levels but no J(Ref.: . . . .)
  - **( )** full rot-vib treatment (number of ν/J levels: . . . .
    Ref.: . . . .)
- **( )** H_2 dissociation (Ref.: . . . .)
- **( )** H_2 formation (Ref.: . . . .)
- **( )** CR heating (Ref.: . . . .)
- **( )** PE heating (Ref.: . . . .)
- **( )** XR heating (Ref.: . . . .)
- **( )** PAH heating (Ref.: . . . .)
- **( )** . . . .
- **( )** . . . .

6 Radiative Transfer

6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

( ) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

- **( )** via simple exponentials (e.g. like in UMIST) (Ref.: . . . .
  . . . .)
- **( )** via biexponentials (e.g. Sternberg & Dalgarno 1995) (Ref.: . . . .
  . . . .)

( ) other (Ref.: . . . .)

Dust Properties

( ) treatment of radiative transfer (Ref.: . . . .)

( ) grain size distribution (Ref.: . . . .)

( ) extinction/scattering law in UV(normalized to A_V(Ref.: . . . .)

( ) albedo (Ref.: . . . .)

( ) scattering function (Eq./Ref.: . . . .)

Shielding of H_2

( ) No

( ) shielding factors (Ref.: . . . .)

( ) single line Ref.: . . . .)

( ) detailed solution (Ref.: . . . .)

Shielding of CO

( ) No

( ) shielding factors (Ref.: . . . .)

( ) single line Ref.: . . . .)

( ) detailed solution (Ref.: . . . .)

( ) Isotope selective photodissociation(Ref.: . . . .)

UV Profile Function for absorption lines (H_2/CO/...)

( ) Gaussian (doppler parameter: . . . .)

( ) Voigt

( ) Box (width: . . . .)

( ) other (Ref.: . . . .)

6.2 Radiative Transfer in Cooling Lines

Method:

( ) Escape probability (Ref.: . . . .
$\beta(\vec{r}) =$ . . . .)

( ) other . . . .

( ) Solution of RT equation in given geometry

( ) IR pumping (e.g. OI) (Ref.: . . . .)

Remarks . . . .)

Cooling Lines included:

- **( )** O (63μ,146μ, ...)
- **( )** ^{12}CO rotational lines (up to J:........)
- **( )** $^{12}C^{+}$ (158 μ)
- **( )** ^{12}C (610 μ,370 μ, ...)
- **( )** Si^{+} (35 μ)
- **( )** ^{13}CO rotational lines (up to J:........)
- **( )** OH rotational lines (up to J:........)
- **( )** H_2O rotational lines (up to J:........)
- **( )** . . . .
- **( )** . . . .

6.3 Radiative Transfer of Observable Line Intensities

Method:

- **( )** Escape probability (Ref.: . . . .
  $\beta(\vec{r}) =$ . . . .)
- **( )** other . . . .
- **( )** no separate treatment from cooling lines (fully self-consistent)

( ) Solution of RT equation in given geometry

Remarks . . . .)

Lines included:

- **( )** O (no. of lines:...........)
- **( )** C (no. of lines:...........)
- **( )** C^{+} (no. of lines:...........)
- **( )** CO (no. of lines:...........)
- **( )** ^{13}CO (no. of lines:...........)
- **( )** $C^{18}O$ (no. of lines:...........)
- **( )** $^{13}C^{18}O$ (no. of lines:...........)
- **( )** H_2O (no. of lines:...........)
- **( )** $H_2{}^{18}O$ (no. of lines:...........)
- **( )** other ....(no. of lines:...........)(Ref.: . . . .)
- **( )** other ....(no. of lines:...........)(Ref.: . . . .)
- **( )** other ....(no. of lines:...........)(Ref.: . . . .)

Computed Line Properties:

( ) fully resolved line profiles (remark: . . . .

. . . .)

( ) contiunuum radiation/radiative transfer of HII-regions . . . .

. . . .

( ) intensities at line center (remark: . . . .

. . . .)

( ) line integrated intensities (remark: . . . .

. . . .)

( ) corresponding optical depths (remark: . . . .

. . . .)

Local velocity dispersion/line profile

- **( )** Gaussian (doppler parameter: . . . .)
- **( )** Box (width: . . . .)
- **( )** other (Ref.: . . . .)

( ) antenna characteristics included

- **( )** HPBW $\gtrless$ cloud (. . . .)
- **( )** beam efficiency(. . . .)
- **( )** atmospheric properties (. . . .)
- **( )** particular telescope simulated (. . . .)
- **( )** beam function (. . . .)
- **( )** . . . .

( ) turbulence included (Ref.: . . . .)

( ) . . . .

( ) . . . .

7 Rate Coefficients

Collision Rates

( ) H-H (Ref.: . . . .)
( ) H-H_2(Ref.: . . . .)
( ) H_2-H^+ (Ref.: . . . .)
( ) H_2-*e* (Ref.: . . . .)
( ) H_2-H_2 (Ref.: . . . .)
( ) CO-H (Ref.: . . . .)
( ) CO-H_2 (Ref.: . . . .)
( ) CO-*e* (Ref.: . . . .)
( ) C^+-*e* (Ref.: . . . .)
( ) C^+-H_2 (Ref.: . . . .)
( ) C^+-H (Ref.: . . . .)
( ) OI-*e* (Ref.: . . . .)
( ) OI-H_2 (Ref.: . . . .)
( ) OI-H (Ref.: . . . .)
( ) ...-H (Ref.: . . . .)
( ) ...-H (Ref.: . . . .)
( ) ...-H (Ref.: . . . .)
( ) ...-H_2 (Ref.: . . . .)
( ) ...-H_2 (Ref.: . . . .)
( ) ...-H_2 (Ref.: . . . .)
( ) ...-H_2O (Ref.: . . . .)
( ) ...-H_2O (Ref.: . . . .)
( ) ...-H_2O (Ref.: . . . .)
( ) ...-H_2O (Ref.: . . . .)
( ) dust-H/H_2 (Ref.: . . . .)
( ) dust-... (Ref.: . . . .)
( ) dust-... (Ref.: . . . .)
( ) dust-... (Ref.: . . . .)
( ) PAH-... (Ref.: . . . .)
( ) PAH-... (Ref.: . . . .)
( ) PAH-... (Ref.: . . . .)
( ) PAH-... (Ref.: . . . .)

( ) ...... (Ref.: . . . .)
( ) ...... (Ref.: . . . .)
( ) ...... (Ref.: . . . .)
( ) ...... (Ref.: . . . .)

A-values

( ) CO (Ref.: . . . .
. . . .)
( ) H_2 (Ref.: . . . .
. . . .)
( ) C (Ref.: . . . .
. . . .)
( ) O (Ref.: . . . .
. . . .)
( ) OH (Ref.: . . . .
. . . .)
( ) C^+ (Ref.: . . . .
. . . .)
( ) H_2O (Ref.: . . . .
. . . .)
( ) ......(Ref.: . . . .
. . . .)
( ) ...... (Ref.: . . . .
. . . .)
( ) ...... (Ref.: . . . .
. . . .)

8 Output

( ) abundance profiles over (A_V/depth)

( ) temperature profile over (A_V/depth)

( ) emitted intensities (details at 6.3)

( ) opacities at linecenters (. . . .)

( ) . . . .

( ) . . . .

( ) . . . .

9 Numerics

Gridded variables

- **( )** frequency/wavelength
- **( )** temperature
- **( )** spatial coordinate(s)
- **( )** velocity
- **( )** time
- **( )** . . . .
- **( )** . . . .

Gridding strategies: . . . .

. . . .

. . . .

Numerical method to solve the chemical network: . . . .

. . . .

. . . .

(Ref.: . . . .)

Numerical method to solve the thermal balance: . . . .

. . . .

. . . .

(Ref.: . . . .)

Numerical method to solve the radiative transfer: . . . .

. . . .

. . . .

(Ref.: . . . .)

Description of the iteration schemes . . . .

. . . .

. . . .

. . . .

. . . .

Numerical parameters to tune convergence/computation speed/accuracy

( ) step size (. . . .)
( ) accuracy goal (. . . .)
( ) starting solution (. . . .)
( ) methods for convergence acceleration (. . . .)
( ) parallelized code(. . . .)
( ) . . . .
( ) . . . .

Usage of numerical standard routines/packages

( ) NAG
( ) BLAS
( ) SLATEC
( ) ODEPACK (LSODE)
( ) LINPACK
( ) . . . .
( ) . . . .

10 Misc

Hardware

( ) x86 PC . . . .
( ) SUN . . . .
( ) HP . . . .
( ) DEC . . . .
( ) IBM . . . .
( ) . . . .

Operating System

( ) Linux . . . .
( ) Solaris . . . .
( ) HP-UX . . . .
( ) MacOS . . . .
( ) other UNIX . . . .
( ) MS Windows . . . .
( ) . . . .

Compiler

Fortran

( ) g77
( ) g90
( ) Absoft f77
( ) Absoft f90
( ) Sun Workshop f77
( ) Sun Workshop f90
( ) ....
( ) ....

C/C++

( ) gcc
( ) Sun Workshop C/C++ compiler
( ) ....
( ) ....

( ) other (....)

Memory Requirements (MB): ....

Processor Speed (MHz): ....

Standard computation time for one model: ....

11 Remarks

....

....

....

....

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