PDR COMPARISON WORKSHOP

Summary of PDR Model Characteristics

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Contents

Chapter 1

Participating Models

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HTBKW *D. Hollenbach, A.G.G.M. Tielens, M.G. Burton, M.J. Kaufman, M.G. Wolfire*

KOSMA-tau *A. Sternberg, J. Stutzki, H. Störzer, B. Köster, M. Zilinsky, U. Leuenhagen, S.Jeyakumar, M.Röllig*

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Chapter 2

Aikawa

2.1 Model Identification

Name of the Model : Lee96mod . . . .

List of Authors : H-H. Lee, E. Herbst, Pineau des Forets, E. Roueff, J. Le Bourlot, Y. Aikawa, N. Kuboi . . . .

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Model has been presented/discussed in (Ref.): Lee et al. (1996) . . . .

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Additional Info : Chemical network and solver of the network are from New Standard Model of Eric Herbst. Calculation of CO- and H2 shielding facors is added by Lee et al. (1996). A subroutine to calculate temperature is added by Kuboi, following Tielens & Hollenbach (1985) and Hollenbach, Takahashi & Tielens 1991. . . . .

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2.2 Geometry

( ) spherical

(X) plane-parallel (semi-infinite)

( ) plane-parallel (finite)

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

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

Density

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

2.3 Radiation Field

( ) isotropic[1] (Ref.: . . . .)

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

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

2.3.1 Radiation sources

( ) external source

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

( ) internal source

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

[1] 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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain I_ν.

2.4 Chemistry

(X) time dependant solution(Ref.: Lee et al. 1996 . . . .)

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

Underlying Database

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

extension of database:

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

(X) fixed number of included species (number: 577.........)

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

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

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

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

(X) formation of other molecules on grains (Ref./Eq.: Ruffle & Herbst 2000; Stantcheva, Caselli, Herbst 2001 . . . .)

(X) desorption mechanisms included

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

( ) metallicity effects included

- **( )** scaling law[2] 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.: . . . .)

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

(X) isotopomers included

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

( ) other ....

( ) other ....

2.5 Thermal Balance

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

(X) temperature determined from energy balance

Cooling Functions

- **(X)** gas-grain cooling (Ref.:...)
- **(X)** radiative line cooling (details in section 13.6.2)
- **( )** ....
- **( )** ....

Heating Functions

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

2.6 Radiative Transfer

2.6.1 UV transfer

(X) RT solved for precomputed density and temperature structure

( ) RT solved selfconsistently with chemical and thermal balance = equations

Attenuation of the photodissociation rates

- **(X)** 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.: . . . .)
- **(X)** extinction/scattering law in UV(normalized to = A_V(Ref.: . . . .)
- **( )** albedo (Ref.: . . . .)
- **( )** scattering function (Eq./Ref.: . . . .)

Shielding of H_2

- **( )** No
- **(X)** shielding factors (Ref.: Lee et al. 1996 . . . .)
- **( )** single line Ref.: . . . .)
- **( )** detailed solution (Ref.: . . . .)

Shielding of CO

- **( )** No
- **(X)** shielding factors (Ref.: Lee et al. 1996 . . . .)
- **( )** 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.: . . . .)

2.6.2 Radiative Transfer in Cooling Lines

Method:

- **(X)** Escape probability (Ref.: de Jong, Dalgarno, & Boland 1980 . . . .
  $\beta(\vec{r}) = 3D$ . . . .)
- **( )** other . . . .

( ) Solution of RT equation in given geometry

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

Remarks . . . .)

Cooling Lines included:

- **(X)** O (63μ,146μ, ...)
- **(X)** ^{12}CO rotational lines (up to J: 6)
- **(X)** $^{12}C^{+}$ (158 μ)
- **(X)** ^{12}C (610 μ,370 μ,230 μ . . . .)
- **( )** Si^{+} (35 μ)
- **(X)** ^{13}CO rotational lines (up to J:........)
- **( )** OH rotational lines (up to J:........)
- **( )** H_2O rotational lines (up to J:........)
- **( )** . . . .
- **( )** . . . .

2.6.3 Radiative Transfer of Observable Line Intensities

Method:

- **( )** Escape probability (Ref.: . . . .
  $\beta(\vec{r}) = 3D$ . . . .)
- **( )** other . . . .
- **( )** no separate treatment from cooling lines (fully self-consistent)

( ) Solution of RT equation in given geometry

Remarks . . . .)

Lines included:

- **(X)** O (no. of lines: 2)
- **(X)** C (no. of lines: 3)
- **(X)** C^{+} (no. of lines: 1)

(X) CO (no. of lines: 6)
( ) ^{13}CO (no. of lines: scaled from 12CO)
( ) 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.: ....)

( ) ....

( ) ....

2.7 Rate Coefficients

Collision Rates

- **( )** H-H (Ref.: collision rates are taken from Warin et al. 1996 . . . .)
- **( )** 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.: . . . .
. . . .)

2.8 Output

(X) abundance profiles over (A_V/depth)

(X) temperature profile over (A_V/depth)

( ) emitted intensities (details at 13.6.3)

( ) opacities at linecenters (. . . .)

( ) . . . .

( ) . . . .

( ) . . . .

2.9 Numerics

Gridded variables

( ) frequency/wavelength

( ) temperature

(X) spatial coordinate(s)

( ) velocity

(X) time

( ) ....

( ) ....

Gridding strategies: Spatial coordinate is gridded logarithmically at small Av. At large Av, it is gridded linearly. Time spacing is automatically calculated so that the temporal variation in the abundance is not too large. ....

....

....

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

....

....

(Ref.:...)

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

....

....

(Ref.:...)

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

....

....

(Ref.:...)

Description of the iteration schemes ....

....

....

....

. . . .

Numerical parameters to tune convergence/computation speed/accuracy

- **( )** step size (. . . .)
- **(X)** accuracy goal (10^{-4} . . . .)
- **( )** starting solution (. . . .)
- **( )** methods for convergence acceleration (. . . .)
- **( )** parallelized code(. . . .)
- **( )** . . . .
- **( )** . . . .

Usage of numerical standard routines/packages

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

2.10 Misc

Hardware

- **(X)** x86 PC . . . .
- **(X)** SUN . . . .
- **( )** HP . . . .
- **( )** DEC . . . .
- **( )** IBM . . . .
- **(X)** ALPHA . . . .

Operating System

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

( ) . . . .

Compiler

Fortran

- **( )** g77
- **( )** g90
- **( )** Absoft f77
- **(X)** Absoft f90
- **( )** Sun Workshop f77
- **(X)** Sun Workshop f90
- **( )** . . . .
- **( )** . . . .

C/C++

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

( ) other (. . . .)

Memory Requirements (MB): . . . .

Processor Speed (MHz): 1 GHz . . . .

Standard computation time for one model: $\sim$ 10 hr . . . .

2.11 Remarks

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Chapter 3

Bensch

3.1 Model Identification

Name: Frank Bensch / spherical PDR model . . . .

List of Authors: Herbert Störzer, Benedikt Köster,
Maik Zilinsky, Uwe Leuenhagen, Solei Jeyakumar, Frank Bensch . . . .

Institute: Center for Astrophysics, Cambridge, MA, USA, and
Radioastronomisches Institut der Universität Bonn, Germany . . . .

Contact Email: fbensch@astro.uni-bonn.de . . . .

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

Störzer, Stutzki & Sternberg, A& A 310, 592 (1996) . . . .

Köster (PhD Thesis, U Köln), Köster et al. A&A 284,
545 (1994) . . . .

Zilinsky (PhD Thesis, U Köln), Zilinsky, Störzer & Stutzki, A&A,
358, 723 (2000) . . . .

Jeyakumar & Stutzki (Proceedings SFChem 2002, NRC press, in press)
. . . .

Bensch et al., ApJ, 591, 1913 (2003) . . . .

Additional Info . . . .

3.2 Geometry

(X) spherical

( ) plane-parallel (semi-infinite)

( ) plane-parallel (finite)

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

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

Density

- **(X)** homogeneous
- **(X)** density gradient (Eq.: $n \propto r^{-\alpha}$ $\alpha \geq 0$ . . . .)
- **(X)** velocity field (Eq.: v =const (no velocity gradient) . . . .)
- **( )** time dependant geometry (. . . .)

3.3 Radiation Field

(X) isotropic[1] (Ref.: . . . .)

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

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

3.3.1 Radiation sources

(X) external source

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

( ) internal source

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

[1]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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain I_ν.

3.4 Chemistry

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

(X) stationary solution(Ref.: Störzer, Stutzki & Sternberg (1996), based on Sternberg & Dalgarno (1995))

Underlying Database

- **( )** UMIST95
- **(X)** UMIST99 (modified + extended by ^{13}C, ^{18}O and PAH)
- **( )** NSM
- **(X)** other (additional species: ^{13}C, ^{18}O and PAH)

extension of database:

Ref.: PAH: following Kaufman et al., ApJ 527, 795 (1999) . . . .

Ref.: Isotopologues: following Maik Zilinsky (master thesis, U Köln) and Köster et al. A&A 284, 545 (1994) . . . .

Ref.: . . . .

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

(X) variable number of included species (arbitrary; code designed to model the main H,C,O bearing species and their isotopologues (gas phase only); current chemical network includes H,He,C,O,S,Si,N,Mg,Fe, ^{13}C, ^{18}O and PAHs; up to 113 species and 59 isotopologues)

(X) PAH's included (Ref.: following Kaufman et al. ApJ 527, 813 (1999) . . . .)

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

(X) formation of H_2 on grains (Ref./Eq.: Sternberg & Dalgarno ApJS 99, 565 (1995) Eq. (A7)-(A9) . . . .)

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

( ) desorption mechanisms included

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

(X) metallicity effects included

scaling relation heating/cooling, abundance: $n(z) = z * n_{\mathrm{z=0}}$ $z = 1 =$solar.

- **(X)** scaling law[2] for elemental abundances (Eq./Ref.: $n(z) = z * n_{\mathrm{z=0}}$ . . . .)
- **(X)** scaling law[3] for dust abundance (Eq./Ref.: $n_d(z) = z * n_{\mathrm{d,z=0}}$ . . . .)
- **(X)** scaling law[3] for PAH abundance (Eq./Ref.: $n(z) = z * n_{\mathrm{z=0}}$ . . . .)
- **(X)** metallicity dependant heating rates (Ref.: $\Gamma(z) = z * \Gamma(z = 0)$ . . . .)
- **(X)** metallicity dependant cooling rates (Ref.:$\Lambda(z) = z * \Lambda(z = 0)$ . . . .)

(X) isotoplogues included

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

( ) other . . . .

( ) other . . . .

3.5 Thermal Balance

(X) fixed temperature law (Eq.: T_{gas} =const. . . . .)

(X) temperature determined from energy balance

Cooling Functions

- **(X)** gas-grain heating or cooling (Ref.: Tielens & Hollenbach, ApJ 1985 291, 722 . . . .)
- **(X)** radiative line cooling (details in section 13.6.2)
- **(X)** recombination cooling (Bakes & Tielens, ApJ 427, 822 (1994) Eq. 4) . . . .
- **( )** . . . .

Heating Functions

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

(X) H_2^* vibrational deexcitation

- **( )** single line approximation(Ref.: . . . .)
- **(x)** only ν-levels but no J(Ref.: . . . .)
- **( )** full rot-vib treatment (number of ν/J levels: . . . .
  Ref.: . . . .)

(X) H_2 dissociation (Ref.: . . . .)

(X) H_2 formation (Ref.: . . . .)

(X) CR heating ($\Lambda_{cr} = 61610 \times \zeta$ (cm^{-1}H-particle^{-1} s^{-1}) with CR destruction rate
$\zeta = 5 \times 10^{-17}$ . . . .)

(X) PE heating (Ref.: Bakes & Tielens, 1994, ApJ, 427, 822 . . . .)

( ) XR heating (Ref.: . . . .)

(X) PAH heating (Ref.: included in PE heating term (size distribution considered) . . . .)

( ) . . . .

( ) . . . .

3.6 Radiative Transfer

3.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(X) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

(X) via simple exponentials (Ref.: . . . .
. . . .)

( ) via biexponentials (e.g. Sternberg & Dalgarno 1995) (Ref.: . . . .
. . . .)

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

Dust Properties

(X) treatment of radiative transfer (Ref.: Hollenbach, Takahashi & Tielens, ApJ, 377, 192 (1991))

(X) grain size distribution (PAHs as chemical species: MRN size distribution for $30 \leq N_C \leq 1500$. For photoelectric heating: see Bakes & Tielens, 1994, ApJ, 427, 822)

(X) 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.: . . . .)

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

Shielding of CO

( ) No

(X) shielding factors (Ref.: van Dishoeck & Black, ApJ 334, 771 (1988) . . . .)

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

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

(X) Isotope selective photodissociation(Ref.: van Dishoeck & Black, ApJ 334, 771 (1988) . . . .)

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

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

( ) Voigt

( ) Box (width: . . . .)

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

3.6.2 Radiative Transfer in Cooling Lines

Method:

(X) Escape probability (Ref.: Störzer, Stutzki & Sternberg, A&A 310, 592 (1996) . . . .

$\beta(\vec{r}) =$ . . . .)

( ) other . . . .

( ) Solution of RT equation in given geometry

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

Remarks . . . .)

Cooling Lines included:

(X) O (63μ,146μ, ...)
(X) ^{12}CO rotational lines (up to J: 40);
(X) $^{12}C^{+}$ (158 μ)
(X) ^{12}C (610 μ,370 μ, ...)
(X) Si^{+} (35 μ)
(X) ^{13}CO rotational lines (up to J: 40)
(X) OH rotational lines (approximation, see Hollenbach & McKee ApJS, 41, 555 (1979).)
(X) H_2O rotational lines (approximation, see Neufeld & Melnick ApJ 322, 266 (1987))
( ) . . . .
( ) . . . .

3.6.3 Radiative Transfer of Observable Line Intensities

Method:

( ) Escape probability (Ref.: . . . .
$\beta(\vec{r}) =$ . . . .)
(X) other: ONION, see Gierens, Stutzki & Winnewisser, A&A 259, 271 (1992) . . . .
( ) no separate treatment from cooling lines (fully self-consistent)

( ) Solution of RT equation in given geometry

Remarks . . . .)

Lines included:

(X) O (no. of lines: 3)
(X) C (no. of lines: 3)
(X) C^{+} (no. of lines: 1)
(X) CO (no. of lines: 50)
(X) ^{13}CO (no. of lines: 50)
(X) $C^{18}O$ (no. of lines: 50)
(X) $^{13}C^{18}O$ (no. of lines: 50)
( ) H_2O (no. of lines:...........)
( ) $H_2{}^{18}O$ (no. of lines:...........)
(X) other: HCO^{+} (no. of lines: 16)(Ref.: . . . .)
( ) other ....(no. of lines:...........)(Ref.: . . . .)

( ) other ....(no. of lines:...........)(Ref.: . . . .)

Computed Line Properties:

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

. . . .)

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

. . . .

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

. . . .)

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

. . . .)

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

. . . .)

Local velocity dispersion/line profile

(X) Gaussian (doppler parameter: β adjusted to the PDR model parameter, including thermal and turbulent component . . . .)

( ) Box (width: . . . .)

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

(X) antenna characteristics included

(X) HPBW $\gtrless$ cloud (. . . .)

(X) beam efficiency(. . . .)

(X) atmospheric properties (. . . .)

( ) particular telescope simulated (. . . .)

( ) beam function (. . . .)

( ) . . . .

(X) turbulence included: Gaussian line width > thermal line width . . . .

( ) . . . .

( ) . . . .

3.7 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.: . . . .
. . . .)

3.8 Output

PDR code:

(X) abundance profiles over (A_V/depth) . . . .

(X) column density over (A_V/depth) . . . .

(X) temperature profile over (A_V/depth) . . . .

(X) heating and cooling over (A_V/depth) and the contribution by different processes discussed above . . . .

(X) chemical rates over (A_V/depth) . . . .

ONION code:

(X) line integrated intensity (details at 13.6.3) . . . .

(X) line peak temperature . . . .

(X) line profiles . . . .

(X) opacities at linecenters . . . .

( ) . . . .

3.9 Numerics

Gridded variables

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

Gridding strategies: . . . .

Adaptive grid, with an pre-defined upper limit for the total number of shells (typ. $N_{\text{shell}} < 400$). . . . .

. . . .

Numerical method to solve the chemical network: rate equations solved using Newton-Raphson method

(Sternberg & Dalgarno, 1995).

. . . .

. . . .

. . . .

(Ref.: Numerical Recipes, Press et al. . . . .)

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

. . . .

. . . .

(Ref.:)

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

In PDR model (in order to calculate the cooling by line emission): escape probability method . . . .

. . . .

(Ref.: Störzer, Stutzki & Sternberg (1996) . . . .)

Description of the iteration schemes . . . .

. . . .

. . . .

. . . .

. . . .

Numerical parameters to tune convergence/computation speed/accuracy

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

Usage of numerical standard routines/packages: code is self-contained; uses subroutines from the Numerical Recipes in F

( ) NAG
( ) BLAS
( ) SLATEC
( ) ODEPACK (LSODE)
( ) LINPACK
(X) Numerical Recipes in Fortran . . . .
( ) . . . .

3.10 Misc

Hardware

- **(X)** x86 PC . . . .
- **(X)** SUN . . . .
- **(X)** HP . . . .
- **( )** DEC . . . .
- **( )** IBM . . . .
- **( )** . . . .

Operating System

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

Compiler

- **Fortran**
  - **(X)** g77
  - **(X)** g90
  - **( )** Absoft f77
  - **( )** Absoft f90
  - **(X)** Sun Workshop f77
  - **(X)** Sun Workshop f90
  - **( )** . . . .
  - **( )** . . . .
- **C/C++**
  - **( )** gcc
  - **( )** Sun Workshop C/C++ compiler
  - **( )** . . . .
  - **( )** . . . .
- **( )** other (. . . .)

Memory Requirements (MB): $< 10^2$ . . . .

Processor Speed (MHz): $>$a few 10^2 . . . .

Standard computation time for one model: between 1 hrs and 1 day, depending on the number of species included . . . .

3.11 Remarks

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....

....

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....

....

Chapter 4

CLOUDY

4.1 Model Identification

Name of the Model: Cloudy

List of Authors: Gary J. Ferland, Peter van Hoof, Nick P. Abel, Gargi Shaw

Institute: University of Kentucky (USA), Queen's University Belfast (Northern Ireland)

Contact Email: gary@uky.edu, p.van-hoof@qub.ac.uk, npabel2@uky.edu, gshaw@pa.uky.edu

Model has been presented/discussed in (Ref.): PASP 110, 761

Hazy, see www.nublado.org

. . . .

Additional Info . . . .

. . . .

. . . .

. . . .

4.2 Geometry

(X) spherical

(X) plane-parallel (semi-infinite)

(X) plane-parallel (finite)

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

(X) other (circumstellar disk)

Density

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

4.3 Radiation Field

( ) isotropic[1] (Ref.: . . . .)

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

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

4.3.1 Radiation sources

(X) external source

- **(X)** Habing field
- **(X)** Draine field
- **(X)** Other (optional star)
- **(X)** detailed spectral energy distribution (Ref.:Hazy)

( ) internal source

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

4.4 Chemistry

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

(X) advection flow

(X) stationary solution(Ref.: Hazy)

Underlying Database

[1]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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain $\bar{I}_\nu$.

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

extension of database:

Ref.: Hollenbach and Mckee 1979, ApJ, 41, 555
Ref.: Galli and Palla 1998, A&A, 335, 403
Ref.: Stancil, Lepp and Dalgarno 1998, ApJ, 509, 1
Ref.: Tielens and Hollanbach 1985, ApJ, 291, 722
Ref.: Hollenbach and Mckee 1989, ApJ, 342, 306
Ref.: Miller et.al. 1997, A&AS, 121,139
Ref.: Maloney et.al. 1996,ApJ, 466, 561

(X) fixed number of included species (number: 33)

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

(X) PAH's included (Ref.:Volk, private communication)

(X) depletion on grains/ice included (Ref.: Hazy, depletion of heavy elements on grains are included.)

(X) formation of H_2 on grains (Ref./Eq.: $3 \times 10^{-18} T^{1/2}$)

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

( ) desorption mechanisms included

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

(X) metallicity effects included

- **(X)** scaling law[2] for elemental abundances (Eq./Ref.: Hazy)
- **(X)** scaling law[3] for dust abundance (Eq./Ref.: Hazy)
- **(X)** scaling law[3] for PAH abundance (Eq./Ref.: Hazy)
- **(X)** metallicity dependant heating rates (Ref.: Hazy)
- **(X)** metallicity dependant cooling rates (Ref.: Hazy)

(X) isotopomers included

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

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

( ) other ....

( ) other ....

4.5 Thermal Balance

(X) fixed temperature law (Eq.: Constant temperature law for constant temperature model)

(X) temperature determined from energy balance

Cooling Functions

- **(X)** gas-grain cooling (Ref.: Hazy)
- **(X)** radiative line cooling (details in section 13.6.2)
- **(X)** radiative recombination
- **( )** ....

Heating Functions

- **(X)** H_2^* vibrational deexcitation
  - **(X)** single line approximation(Ref.:.................................)
  - **( )** only ν-levels but no J(Ref.:.......................................)
  - **(X)** full rot-vib treatment (number of ν/J levels: 1893 – X, B, C) Ref.: Hazy)
- **(X)** H_2 dissociation (Ref.: Detail treatment of Solomon process)
- **(X)** H_2 formation (Ref.: Hazy)
- **(X)** CR heating (Ref.: Hazy)
- **(X)** PE heating (Ref.: Weingartner & Draine 2001, ApJS, 134, 263)
- **(X)** XR heating (Ref.: Hazy)
- **(X)** PAH heating (Ref.: Weingartner & Draine 2001, ApJS, 134, 263)
- **(X)** photoionization of C, Si, etc.
- **(X)** gas-grain collisions (Ref.: Hazy)
- **(X)** turbulence heating

4.6 Radiative Transfer

4.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(X) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

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

Dust Properties

- **(X)** treatment of radiative transfer (Ref.: Hazy)
- **(X)** grain size distribution (Ref.: Hazy)
- **(X)** extinction/scattering law in UV (normalized to A_V, Ref.: Hazy, code used optical properties determined from Mie theorem and spherical grains)
- **(X)** albedo (Ref.: Hazy)
- **(X)** scattering function (Eq./Ref.: What is the difference between scattering function and scattering law?)

Shielding of H_2

- **( )** No
- **(X)** shielding factors (Ref.: . . . .)
- **(X)** single line Ref.: . . . .)
- **(X)** detailed solution (Ref.: Hazy)

Shielding of CO

- **( )** No
- **( )** shielding factors (Ref.: . . . .)
- **(X)** single line Ref.: van Dishoeck, E.F., & Black, J.H., 1988, ApJ, 334, 771
- **( )** detailed solution (Ref.: . . . .)
- **( )** Isotope selective photodissociation(Ref.: . . . .)

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

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

4.6.2 Radiative Transfer in Cooling Lines

Method:

- **(X)** Escape probability (Ref.:Hazy
  $\beta(\vec{r}) =$ . . . .)
- **( )** other . . . .

(X) Solution of RT equation in given geometry

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

Remarks . . . .)

Cooling Lines included:

- **(X)** O (63μ, 146μ, 6300A^0, 6363A^0, 5577A^0)
- **(X)** ^{12}CO rotational lines (up to J: 20)
- **(X)** $^{12}C^+$ (158 μ, 1020A^0, 1335A^0)
- **(X)** ^{12}C (610 μ, 370 μ, 1.069μ, 6828A^0, 1315A^0, 1166A^0)
- **(X)** Si^+ (35 μ, 1814A^0, 1531A^0, 1308A^0, 1263A^0)
- **(X)** ^{13}CO rotational lines (up to J: 20)
- **( )** OH rotational lines (up to J:........)
- **( )** H_2O rotational lines (up to J:........)
- **(X)** H_2 rotational lines
- **(X)** HD rotational lines
- **(X)** O 6300 $\AA$ metastable lines
- **(X)** Ly α metastable lines
- **(X)** Fe 24μ, 34μ), $Fe^+(26\mu, 35.4\mu)$
- **( )** H_2 rot-vib

4.6.3 Radiative Transfer of Observable Line Intensities

Method:

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

( ) Solution of RT equation in given geometry

Remarks . . . .)

Lines included:

(X) O (no. of lines: more than 10)
(X) C (no. of lines: more than 10)
(X) C^+ (no. of lines: more than 10)
(X) CO (no. of lines: 40)
(X) ^{13}CO (no. of lines: 20)
( ) $C^{18}O$ (no. of lines:...........)
( ) $^{13}C^{18}O$ (no. of lines:...........)
( ) H_2O (no. of lines:...........)
( ) $H_2{}^{18}O$ (no. of lines:...........)
(X) H_2
(X) Si^+
(X) SiI
(X) SI,SII
(X) SiIFeI,FeII

Computed Line Properties:

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

. . . .)

(X) contiunuum radiation/radiative transfer of HII-regions (remark: Hybrid, “Outward-only” and “On the spot”

Details in Hazy.

(X) intensities at line center (remark: Only 21cm, Details in Hazy

. . . .)

(X) line integrated intensities (remark: Details in Hazy

. . . .)

(X) corresponding optical depths (remark: Details in Hazy

. . . .)

Local velocity dispersion/line profile

(X) Gaussian (doppler parameter: Details in Hazy)
( ) Box (width: . . . .)
( ) other (Ref.: . . . .)

( ) antenna characteristics included

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

(X) turbulence included (Ref.: Hazy)

( ) . . . .

( ) . . . .

4.7 Rate Coefficients

Collision Rates

- **(X)** H-H (Ref.: Hazy)
- **(X)** H-H_2(Ref.: Le Bourlot et. al 1999, MNRAS, 305, 802)
- **(X)** H_2-H^+ (Ref.: Gerlich 1990, J.Chem.Phys., 92,2377)
- **(X)** H_2-e (Ref.: Stibbe & Tennyson 1999, ApJ, 516, 371)
- **(X)** H_2-H_2 (Ref.: Le Bourlot et. al 1999, MNRAS, 305, 802)
- **(X)** CO-H (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)
- **(X)** CO-H_2 (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)
- **(X)** CO-e (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)
- **(X)** C^+-e (Ref.: Pequignot, Petitjean & Boisson 1991, A&A, 251, 680)
- **(X)** C^+-H_2 (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)
- **(X)** C^+-H (Ref.: Hollenbach & Tielens 1985, ApJ, 291, 722)
- **(X)** OI-e (Ref.: Bell et al. 1998, MNRAS 293, L83, for $T_e \leq 3000$K
  Berrington, K.A. 1988, J.Phys.B, 21, 1083, for $T_e > 3000$K
- **(X)** OI-H (Ref.: Launay & Roueff 1977, AA 56, 289)
- **(X)** OI-H^+ (Ref: Pequignot, D. 1990, A&A 231, 499)
- **(X)** OI-H_2 (Ref.: Jaquet et al. 1992, J.Phys.B 25, 285)
- **(X)** OI-He (Ref.: Monteiro & Flower 1987, MNRAS 228, 101)
- **(X)** OH-H (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)
- **(X)** H^--H (Ref.: Launay et.al. 1991, A&A, 252, 842)
- **( )** -H (Ref.: . . . .)

( ) ...-H_2 (Ref.: . . . .)

( ) ...-H_2 (Ref.: . . . .)

(X) OH-H_2 (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)

(X) C-H_2O (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)

(X) e-H_2O (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)

(X) H-H_2O (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)

(X) O-H_2O (Ref.: Hollenbach & Mckee 1989, ApJ, 342, 306)

(X) dust-H/H_2 (Ref.: Cazaux & Tielens 2002, ApJ, 575, L29)

(X) dust-any (Ref.: Weingartner & Draine 2001, ApJS, 134, 263)

( ) dust-... (Ref.: . . . .)

( ) dust-... (Ref.: . . . .)

( ) PAH-any (Ref.: Weingartner & Draine 2001, ApJS, 134, 263)

( ) PAH-... (Ref.: . . . .)

( ) PAH-... (Ref.: . . . .)

( ) PAH-... (Ref.: . . . .)

( ) C-e

( ) Si^+-H

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

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

A-values

(X) CO (Ref.: rigid rotator, groung v
. . . .)

(X) H_2 (Ref.: Abgrall, H., Roulff, E., & Drira, I. 2000, A&AS, 141,297
Wolnievicz, L., Simbotin, I., Dalgarno, A. 1998, ApJs, 115, 293)

(X) C (Ref.: Hazy
. . . .)

(X) O (Ref.: Hazy
. . . .)

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

(X) C^+ (Ref.: Hazy
. . . .)

( ) H_2O (Ref.: . . . .
. . . .)

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

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

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

4.8 Output

(X) abundance profiles over (A_V/depth)

(X) temperature profile over (A_V/depth)

(X) emitted intensities (details at 13.6.3)

( ) opacities at linecenters (. . . .)

(X) Heating and cooling rates

(X) column density over (A_V/depth)

( ) excitation diagram of H_2

4.9 Numerics

Gridded variables

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

Gridding strategies: multi-grid-line transfer on fine grid,

continuum transfer on course grid

. . . .

Numerical method to solve the chemical network: Linearization scheme

. . . .

. . . .

(Ref.: . . . .)

Numerical method to solve the thermal balance: Linearization scheme

. . . .

. . . .

(Ref.: . . . .)

Numerical method to solve the radiative transfer: Linearization scheme

. . . .

. . . .

(Ref.: . . . .)

Description of the iteration schemes: Linearization scheme

. . . .

. . . .

. . . .

. . . .

Numerical parameters to tune convergence/computation speed/accuracy

- **(X)** step size (adaptive)
- **(X)** accuracy goal (1%)
- **( )** starting solution (. . . .)
- **( )** methods for convergence acceleration (. . . .)
- **( )** parallelized code(. . . .)
- **( )** . . . .
- **( )** . . . .

Usage of numerical standard routines/packages

- **( )** NAG
- **( )** BLAS
- **( )** SLATEC
- **( )** ODEPACK (LSODE)
- **( )** LINPACK
- **(X)** LAPACK
- **( )** . . . .

4.10 Misc

Hardware

- **( )** x86 PC . . . .
- **( )** SUN . . . .
- **( )** HP . . . .
- **( )** DEC . . . .
- **( )** IBM . . . .
- **(X)** Any machine with ANSI standard

Operating System

- **( )** Linux . . . .
- **( )** Solaris . . . .
- **( )** HP-UX . . . .
- **( )** MacOS . . . .
- **( )** other UNIX . . . .
- **( )** MS Windows . . . .
- **(X)** Any machine with ANSI standard

Compiler

- **Fortran**
  - **( )** g77
  - **( )** g90
  - **( )** Absoft f77
  - **( )** Absoft f90
  - **( )** Sun Workshop f77
  - **( )** Sun Workshop f90
  - **( )** . . . .
  - **( )** . . . .
- **C/C++**
  - **( )** gcc
  - **( )** Sun Workshop C/C++ compiler
  - **( )** cc
  - **(X)** C compiler
- **( )** other (. . . .)

Memory Requirements (MB): 188

Processor Speed (MHz): 1000

Standard computation time for one model: 7000 sec(CPU time)

4.11 Remarks

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Chapter 5

COSTAR

5.1 Model Identification

Name of the Model COSTAR . . . .

List of Authors Kamp, I., Bertoldi, F., van Zadelhoff, G.-J. . . . .

Institute Leiden Observatory . . . .

Contact Email kamp@strw.leidenuniv.nl . . . .

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

Kamp & Bertoldi (2000) . . . .

Kamp & van Zadelhoff (2001) . . . .

Additional Info . . . .

code was initially developed for circumstellar disks . . . .

. . . .

. . . .

5.2 Geometry

( ) spherical

( ) plane-parallel (semi-infinite)

( ) plane-parallel (finite)

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

(x) other (Ref.: Kamp & Bertoldi (2000) . . . .)

Density

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

5.3 Radiation Field

( ) isotropic[1] (Ref.: . . . .)

(x) uni-directional (Ref.: Kamp & Bertoldi (2000) . . . .)

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

5.3.1 Radiation sources

( ) external source

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

( ) internal source

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

5.4 Chemistry

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

(x) stationary solution(Ref.: Kamp & Bertoldi (2000) . . . .)

Underlying Database

- **( )** UMIST95
- **( )** UMIST99

[1]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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain $\bar{I}_\nu$.

- **( )** NSM
- **(x)** other (Ref.: Kamp (1998) . . . .)

extension of database:

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

(x) fixed number of included species (number: 48......)

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

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

(x) depletion on grains/ice included (Ref.: CO: Kamp & Bertoldi (2000) . . . .)

(x) formation of H_2 on grains (Ref./Eq.: $R_{form} = 3\,10^{-17}\sqrt{T/100\,K}$ Kamp & Bertoldi (2000) . . . .)

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

(x) desorption mechanisms included

- **( )** photoevaporation
- **(x)** thermal desorption
- **( )** CR spot heating
- **( )** grain-grain collisions
- **( )** grain sputtering

(x) metallicity effects included

- **( )** scaling law[2] 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

---

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

( ) . . . .

( ) . . . .

( ) other . . . .

( ) other . . . .

5.5 Thermal Balance

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

(x) temperature determined from energy balance

Cooling Functions

- **(x)** gas-grain cooling (Ref.: Burke & Hollenbach (1983) . . . .)
- **(x)** radiative line cooling (details in section 13.6.2)
- **( )** . . . .
- **( )** . . . .

Heating Functions

- **(x)** H_2^* vibrational deexcitation
  - **(x)** single line approximation(Ref.: Tielens & Hollenbach (1985) . . . . . .)
  - **( )** only ν-levels but no J(Ref.: . . . .)
  - **( )** full rot-vib treatment (number of ν/J levels: . . . .
    Ref.: . . . .)
- **(x)** H_2 dissociation (Ref.: Stephens & Dalgarno (1973) . . . .)
- **(x)** H_2 formation (Ref.: Black & Dalgarno (1976) . . . .)
- **(x)** CR heating (Ref.: Clavel et al. (1978), Hollenbach & McKee (1989) . . . .)
- **(x)** PE heating (Ref.: Tielens & Hollenbach (1985) . . . .)
- **( )** XR heating (Ref.: . . . .)
- **( )** PAH heating (Ref.: . . . .)
- **(x)** C ionisation (Ref.: Black (1987) . . . .)
- **( )** . . . .

5.6 Radiative Transfer

5.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(x) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

(x) via simple exponentials (e.g. like in UMIST) (Ref.: ....)

(x) via biexponentials (e.g. Sternberg & Dalgarno 1995) (Ref.: ....)

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

Dust Properties

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

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

(x) extinction/scattering law in UV(normalized to A_V(Ref.: Cardelli, Clayton & Mathis (1989) ....)

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

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

Shielding of H_2

( ) No

(x) shielding factors (Ref.: Draine & Bertoldi (1996) ....)

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

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

Shielding of CO

( ) No

(x) shielding factors (Ref.: Kamp & Bertoldi (2000) ....)

( ) 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.: ....)

5.6.2 Radiative Transfer in Cooling Lines

Method:

- **(x)** Escape probability (Ref.: Tielens & Hollenbach (1985) . . . .
  $\beta(\tau) = (1 - \exp(-2.34\tau))/(4.68\tau), \tau < 7$ and
  $\beta(\tau) = 1/(4\tau\sqrt{ln(\tau/\sqrt{\pi})}), \tau \geq 7$ . . . .)
- **( )** other . . . .

( ) Solution of RT equation in given geometry

(x) IR pumping (e.g. OI) (Ref.: Kamp & van Zadelhoff (2001) . . . .)

Remarks . . . .)

Cooling Lines included:

- **(x)** O (63μ,146μ,44μ)
- **(x)** ^{12}CO rotational lines (up to J: 25)
- **(x)** $^{12}C^+$ (158 μ)
- **(x)** ^{12}C (610 μ,370 μ, 230 μ)
- **( )** Si^+ (35 μ)
- **( )** ^{13}CO rotational lines (up to J:........)
- **( )** OH rotational lines (up to J:........)
- **( )** H_2O rotational lines (up to J:........)
- **(x)** CH rotational lines . . . .
- **(x)** OI 6300 μ, Lyα . . . .

5.6.3 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.: . . . .)

( ) . . . .

( ) . . . .

5.7 Rate Coefficients

Collision Rates

( ) H-H (Ref.: . . . .)

( ) H-H_2(Ref.: . . . .)

( ) H_2-H^+ (Ref.: . . . .)

( ) H_2-*e* (Ref.: . . . .)

( ) H_2-H_2 (Ref.: . . . .)

(x) CO-H (Ref.: Chu & Dalgarno (1975) . . . .)

(x) CO-H_2 (Ref.: Schinke et al. (1985) . . . .)

(x) CO-*e* (Ref.: . . . .)

(x) C^+-*e* (Ref.: Mendoza (1983); Keenan et al. (1986) . . . .)

(x) C^+-H_2 (Ref.: Flower (1977) . . . .)

(x) C^+-H (Ref.: Flower (1977) . . . .)

(x) OI-*e* (Ref.: Liseau et al. (1999) . . . .)

(x) OI-H_2 (Ref.: Liseau et al. (1999) . . . .)

(x) OI-H (Ref.: Liseau et al. (1999) . . . .)

(x) C-H_2 (Ref.: Schroeder et al. (1991) . . . .)

(x) C-H (Ref.: Launay & Roueff (1977) . . . .)

( ) ...-H (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

(x) CO (Ref.: . . . .
. . . .)

( ) H_2 (Ref.: . . . .
. . . .)

(x) C (Ref.: . . . .
. . . .)

(x) O (Ref.: . . . .
. . . .)

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

(x) C^+ (Ref.: . . . .
. . . .)

( ) H_2O (Ref.: . . . .
. . . .)

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

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

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

5.8 Output

(x) abundance profiles over (A_V/depth)

(x) temperature profile over (A_V/depth)

( ) emitted intensities (details at 13.6.3)

( ) opacities at linecenters (. . . .)

( ) . . . .

( ) . . . .

( ) . . . .

5.9 Numerics

Gridded variables

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

Gridding strategies: . . . .

logarithmic in A_V . . . .

. . . .

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

modified Newton-Raphson . . . .

. . . .

(Ref.: . . . .)

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

modified Riddr's method . . . .

. . . .

(Ref.: . . . .)

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

....

....

(Ref.: ....)

Description of the iteration schemes ....

....

....

....

....

Numerical parameters to tune convergence/computation speed/accuracy

- **( )** step size (....)
- **(x)** accuracy goal (0.1% for T$_gas$)
- **( )** starting solution (....)
- **( )** methods for convergence acceleration (..................................)
- **( )** parallelized code(....)
- **( )** ....
- **( )** ....

Usage of numerical standard routines/packages

- **( )** NAG
- **( )** BLAS
- **( )** SLATEC
- **( )** ODEPACK (LSODE)
- **( )** LINPACK
- **(x)** NUMERICAL RECIPES
- **( )** ....

5.10 Misc

Hardware

- **(x)** x86 PC ....
- **( )** SUN ....
- **( )** HP ....

( ) DEC . . . .

( ) IBM . . . .

( ) . . . .

Operating System

(x) Linux . . . .

( ) Solaris . . . .

( ) HP-UX . . . .

( ) MacOS . . . .

( ) other UNIX . . . .

( ) MS Windows . . . .

( ) . . . .

Compiler

Fortran

- **( )** g77
- **( )** g90
- **( )** Absoft f77
- **(x)** Absoft f90
- **( )** Sun Workshop f77
- **( )** Sun Workshop f90
- **( )** . . . .
- **( )** . . . .

C/C++

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

( ) other (. . . .)

Memory Requirements (MB): . . . .

Processor Speed (MHz): 500 . . . .

Standard computation time for one model: $\sim$ 13 min . . . .

5.11 Remarks

....

....

....

....

....

....

....

....

Chapter 6

HTBKW

6.1 Model Identification

Name of the Model : “chemh2” . . . .

List of Authors Michael J. Kaufman[1], Mark G. Wolfire[2], David J. Hollenbach[3] . . . .

Institute [1]San Jose State University, [2]University of Maryland, College Park, [3]NASA/Ames Research Center . . . .

Contact Email kaufman@ism.arc.nasa.gov, mwolfire@astro.umd.edu . . . .

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

Kaufman, Wolfire, Hollenbach, & Luhman 1999, ApJ, 527, 795 . . . .

Hollenbach, Takahashi, & Tielens 1991, ApJ, 377, 192 . . . .

Wolfire, Tielens, & Hollenbach 1990, ApJ, 358, 116 . . . .

Burton, Hollenbach, & Tielens, 1990, ApJ, 365, 630

Tielens, & Hollenbach 1985, ApJ 291, 722 . . . .

Additional Info Additional Updates in: . . . .

Wolfire, Hollenbach, McKee, Tielens, & Bakes 1995, ApJ, 443, 152 . . . .

Wolfire, McKee, Hollenbach, & Tielens 2003, ApJ, 587, 278 . . . .

. . . .

6.2 Geometry

( ) spherical

(X) plane-parallel (semi-infinite)

(X) plane-parallel (finite)

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

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

Density

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

6.3 Radiation Field

( ) isotropic[1] (Ref.: ....)

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

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

6.3.1 Radiation sources

(X) external source

- **(X)** Habing field
- **(X)** Draine field (For localISRF we use the integrated energy density of the Draine field $G_0 = 1.7$).
- **( )** Other (Ref.: ....)
- **( )** detailed spectral energy distribution (Ref.:..)

( ) internal source

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

[1]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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain I_ν.

6.4 Chemistry

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

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

Underlying Database

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

extension of database:

Ref.:Tielens & Hollenbach 1985, ApJ, 291, 722 . . . .
Ref.:Hollenbach & McKee 1989, ApJ, 342, 306 . . . .
Ref.:Hollenbach, Takahashi, & Tielens 1991, ApJ, 377, 192 . . . .
Ref.:Spaans, Tielens, van Dishoeck, & Bakes 1994, ApJ, 437, 270 . . . .
Ref.:Wolfire, McKee, Hollenbach, & Tielens 2003, ApJ, 587, 278 . . . .

(X) fixed number of included species (number: 46)

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

(X) PAH's included (Ref.:Wolfire, et al. 1995, ApJ, 443, 152; Wolfire, et al. 2003, ApJ, 587 278; Bakes & Tielens 1994, ApJ, 427, 822; Draine & Sutin 1987, ApJ, 320, 803 . . . .)

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

(X) formation of H_2 on grains Ref./Eq.: Kaufman et al. 1999, ApJ, 527, 795 . . . .

Rate $= 3.0 \times 10^{-17} n n_{\mathrm{H}}$ cm^{-3} s^{-1} . . . .

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

( ) desorption mechanisms included

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

(X) metallicity effects included

- **(X)** scaling law[2] for elemental abundances (Eq./Ref.: Independently variable .)

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

- **(X)** scaling law[3] for dust abundance (Eq./Ref.:Independently variable . . . .)
- **(X)** scaling law[3] for PAH abundance (Eq./Ref.:Independently variable . . . .)
- **(X)** metallicity dependant heating rates (Ref.: . . . .)
- **(X)** metallicity dependant cooling rates (Ref.: . . . .)

( ) isotopomers included

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

( ) other . . . .

( ) other . . . .

6.5 Thermal Balance

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

(X) temperature determined from energy balance

Cooling Functions

- **(X)** gas-grain cooling (Ref.:Hollenbach & McKee 1989, ApJ, 342, 306 . . . .)
- **(X)** radiative line cooling (details in section 13.6.2)
- **( )** . . . .
- **( )** . . . .

Heating Functions

- **(X)** H_2^* vibrational deexcitation
  - **(X)** single line approximation(Ref.:Burton, Hollenbach, & Tielens 1990, ApJ, 365, 620 . . . .)
  - **( )** only ν-levels but no J(Ref.: . . . .)
  - **(-)** full rot-vib treatment (number of ν/J levels: - In process adopted from Le Bourlot PDR code . . . .)
- **(X)** H_2 dissociation (Ref.:Tielens & Hollenbach 1985, ApJ, 291, 722 . . . .
  [Le Bourlot PDR code in process] . . . .)
- **(-)** H_2 formation (Ref.: - In process adopted from Le Bourlot PDR code . . . . . .)

- **(X)** CR heating (Ref.:Wolfire, et al. 1995, ApJ, 443, 152, Maloney, Hollenbach, & Tielens 1996, ApJ, 466, 561 . . . .)
- **(X)** PE heating (Ref.:Bakes & Tielens 1994, ApJ, 427, 822; Wolfire et al. 2003, ApJ, 587, 278 . . . .)
- **(X)** XR heating (Ref.:Wolfire et al. 1995, ApJ, 443, 152 . . . .)
- **(X)** PAH heating (Ref.:Bakes & Tielens 1994, ApJ, 427, 822; Wolfire et al. 2003, ApJ, 587, 278 . . . .)
- **( )** . . . .
- **( )** . . . .

6.6 Radiative Transfer

6.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(X) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

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

Dust Properties

- **(X)** treatment of radiative transfer [for dust temperature] (Ref.:Hollenbach, Takahashi, & Tielens 1991, ApJ, 377, 192 . . . .)
- **( )** grain size distribution (Ref.: . . . .)
- **(X)** extinction/scattering law in UV normalized to A_V(Ref. Roberge, Dalgarno, & Flannery 1981, ApJ, 243, 817; Black & Dalgarno 1977, ApJS, 34, 405)
- **( )** albedo (Ref.: . . . .)
- **( )** scattering function (Eq./Ref.: . . . .)

Shielding of H_2

- **(X)** Unshielded rate from Abgrall, H. et al. 1992, AA, 235, 525
- **(X)** shielding factors (Ref.:Draine & Bertoldi 1996, ApJ, 468, 269 . . . .)
- **( )** single line Ref.: . . . .)
- **( )** detailed solution (Ref.: . . . .)

Shielding of CO

(X) Unshielded rate from van Dishoeck & Black 1988, ApJ, 334, 771 . . . .
(X) shielding factors (Ref.:van Dishoeck & Black 1988, ApJ, 334, 771 . . . .)
( ) single line Ref.: . . . .)
( ) detailed solution (Ref.: . . . .)
( ) Isotope selective photodissociation(Ref.: . . . .)

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

(X) Gaussian (doppler parameter: fixed width input parameter . . . .)
( ) Voigt
( ) Box (width: . . . .)
( ) other (Ref.: . . . .)

6.6.2 Radiative Transfer in Cooling Lines

Method:

(X) Escape probability (Ref.:Tielens & Hollenbach 1985, ApJ, 291, 722
de Jong, Dalgarno, & Boland 1980, AA, 91, 68 . . . .
$\beta(\vec{r}) =$ . . . .)
( ) other . . . .

( ) Solution of RT equation in given geometry

(X) IR pumping (e.g. OI) (Ref.:Tielens & Hollenbach 1985, ApJ, 291, 772 . . . .)

Remarks . . . .)

Cooling Lines included:

(X) O (63μm,146μm, ...)
(X) ^{12}CO rotational lines (up to J:20)
(X) $^{12}C^+$ (158 μm)
(X) ^{12}C (610 μm,370 μm, ...)
(X) Si^+ (35 μ)
( ) ^{13}CO rotational lines (up to J:........)
(X) OH rotational lines (up to J:45): Parameterized fit by Uma Gorti and Michael Kaufman
(X) H_2O rotational lines (up to J:165): Parameterized fit by Uma Gorti and Michael Kaufman
(X) Fe (24 μm, 34 μm); Fe^+ (26.0 μm 35.4 μm) . . . .
(X) H_2 thermal excitation of low lying v and j levels . . . .

6.6.3 Radiative Transfer of Observable Line Intensities

Method:

(X) Escape probability (Ref.:Tielens & Hollenbach 1985, ApJ, 291, 722
de Jong, Dalgarno, & Boland 1980, AA, 91, 68 . . . .
$\beta(\vec{r}) =$ . . . .)

( ) other . . . .

(-) no separate treatment from cooling lines (fully self-consistent) Except for HCO^+ and H_2 (full self-consistent treatment of H_2 in process)

( ) Solution of RT equation in given geometry

Remarks . . . .)

Lines included:

(X) O (no. of lines: 9: 3 fine-structure 6 metastable)

(X) C (no. of lines: 6: 3 fine-structure 3 metastable)

(X) C^+ (no. of lines: 2: 1 fine-structure 1 metastable)

(X) CO (no. of lines: 20)

( ) ^{13}CO (no. of lines:...........)

( ) $C^{18}O$ (no. of lines:...........)

( ) $^{13}C^{18}O$ (no. of lines:...........)

(X) H_2O (no. of lines: 1)

( ) $H_2{}^{18}O$ (no. of lines:...........)

(X) other OH...(no. of lines:. 1)

(X) other SiI...........(no. of lines: 6: 3 fine-structure 3 metastable)

(X) other SiII...........(no. of lines: 2: 1 fine-structure 1 metastable)

(X) other SI........(no. of lines: 6: 3 fine-structure 3 metastable)

(X) other SII........(no. of lines: 6: 3 fine-structure 3 metastable)

(X) other FeI........(no. of lines: 6: 3 fine-structure 3 metastable)

(X) other FeII.......(no. of lines: 6: 3 fine-structure 3 metastable)

(X) other HCO^+.......(no. of lines: 20)

Computed Line Properties:

(X) fully resolved line profiles (remark: For ^{12}CO . . . .)

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

. . . .

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

. . . .)

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

. . . .)

(X) corresponding optical depths (remark:Escape probability formalism . . . .

. . . .)

Local velocity dispersion/line profile

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

( ) antenna characteristics included

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

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

( ) . . . .

( ) . . . .

6.7 Rate Coefficients

Collision Rates

- **(X)** H-H (Ref.:Hollenbach & McKee 1989, ApJ, 342, 306 . . . .)
- **(X)** H_2-H(Ref.: Burton, Hollenbach & Tielens 1990, ApJ, 365, 620;
  Draine, Roberge, & Dalgarno 1983, ApJ, 264, 48;
  Hollenbach & McKee 1979, ApJS, 41, 555 . . . .)
- **( )** H_2-H^+ (Ref.: . . . .)
- **(X)** H_2-*e* (Ref.:Burton, Hollenbach & Tielens 1990, ApJ, 365, 620;
  Draine, Roberge, & Dalgarno 1983, ApJ, 264, 485;
  Hollenbach & McKee 1979, ApJS, 41, 555 . . . .)
- **(X)** H_2-H_2 (Ref.: Burton, Hollenbach & Tielens 1990, ApJ, 365, 620;
  Hollenbach & McKee 1979, ApJS, 41, 555 . . . .)

(X) CO-H (Ref.:Tielens & Hollenbach 1985, ApJ, 291, 722
de Jong, Chu, & Dalgarno 1975, ApJ, 199, 69 . . . .)

(X) CO-H_2 (Ref.: Tielens & Hollenbach 1985, ApJ, 291,722
de Jong, Chu, & Dalgarno 1975, ApJ, 199, 69 . . . .)

( ) CO-*e* (Ref.: . . . .)

(X) C^+-*e* (Ref.:Blum & Pradhan 1992, ApJS, 80, 425 . . . .)

(X) C^+-H_2 (Ref.:Flower & Launay 1977, JPhB, 10, 3673 . . . .)

(X) C^+-H (Ref.:Launay & Roueff 1977, JPhB, 10, 879 . . . .)

(X) OI-*e* (Ref.:Péquignot 1990, AA, 231, 499 . . . .)

(X) OI-H_2 (Ref.:Jaquet et al. 1992, JPhB, 25, 285
Spaans, Tielens, van Dishoeck, & Bakes 1994, ApJ, 437, 270 . . . .)

(X) OI-H (Ref.:Péquignot 1990, AA, 231, 499 . . . .)

(X) CI-H (Ref.:Launay & Roueff 1977, AA, 56, 289 . . . .)

( ) ...-H (Ref.: . . . .)

( ) ...-H (Ref.: . . . .)

(X) CI-H_2 (Ref.:Schröeder et al. 1991, JPhB, 24, 2487
Spaans, Tielens, van Dishoeck, & Bakes 1994, ApJ, 437, 270 . . . .)

(X) OH-H_2 (Ref.:Offer & van Dishoeck 1992, MNRAS, 257, 377
(Kaufman + Gorti fit) . . . .)

(X) H_2O-H_2 (Ref.:Phillips, Maluendes, & Green 1996, ApJ, 107, 467
(Kaufman + Gorti fit) . . . .)

( ) ...H_2O (Ref.: . . . .)

( ) ...-H_2O (Ref.: . . . .)

( ) ...-H_2O (Ref.: . . . .)

( ) ...-H_2O (Ref.: . . . .)

(X) dust-H/H_2 (Ref.:Burton, Tielens, & Hollenbach 1992, ApJ, 399 563
Kaufman et al. 1999, ApJ, 527, 795 . . . .)

( ) dust-... (Ref.: . . . .)

( ) dust-... (Ref.: . . . .)

( ) dust-... (Ref.: . . . .)

(X) PAH^--H^+... (Ref.:Wolfire et al. 2003, ApJ, 587, 278 . . . .)

(X) PAH^0-H^+... (Ref.:Wolfire et al. 2003 . . . .)

(X) PAH^0-$h\nu$... (Ref.:Wolfire et al. 2003 . . . .)

(X) PAH^+-*e*... (Ref.:Wolfire et al. 2003 . . . .)

(X) PAH^--$h\nu$...(Ref.:Wolfire et al. 2003 . . . .)

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

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

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

A-values

(X) CO (Ref.:de Jong, Chu, & Dalgarno 1975, ApJ, 199, 69 . . . .
. . . .)

(X) H_2 (Ref.:Turner, Kirby-Docken, & Dalgarno 1977, ApJS, 35, 281 . . . .)
. . . .)

(X) C (Ref.:Galavis, Mendoza, & Zeippen 1997, AA Supp. 123, 159 . . . .

(X) O (Ref.:Galavis, Mendoza, & Zeippen 1997, AA Supp. 123, 159 . . . .

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

(X) C^+ (Ref.:Tielens & Hollenbach 1985 . . . .
. . . .)

( ) H_2O (Ref.: . . . .
. . . .)

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

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

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

6.8 Output

(X) abundance profiles over (A_V/depth)

(X temperature profile over (A_V/depth)

(X) emitted intensities (details at 13.6.3)

(X) opacities at linecenters (. . . .)

( ) . . . .

( ) . . . .

( ) . . . .

6.9 Numerics

Gridded variables

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

Gridding strategies: Small steps at $A_v < 1$ and check for unphysical jumps in CO and H_2 columns. ....

....

....

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

Newton-Raphson method...

....

(Ref.:Tielens & Hollenbach 1985, Tielens & Hagen 1982, AA, 114, 245 ....)

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

Binary Iteration ....

....

(Ref.:Tielens & Hollenbach 1985...)

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

....

....

(Ref.:...)

Description of the iteration schemes ....

Inner loop: chemistry iteration, Outer loop: Temperature/Thermal Balance iteration .

....

....

. . . .

Numerical parameters to tune convergence/computation speed/accuracy

(X) step size (At least 60 points at $A_v < 1$ 200 points total . . . .)

(X) accuracy goal (0.1% in temperature and abundance . . . .)

(X) starting solution (atomic gas . . . .)

( ) methods for convergence acceleration (. . . .)

( ) parallelized code(. . . .)

( ) . . . .

( ) . . . .

Usage of numerical standard routines/packages

( ) NAG

( ) BLAS

( ) SLATEC

( ) ODEPACK (LSODE)

(X) LINPACK

( ) . . . .

( ) . . . .

6.10 Misc

Hardware

(X) x86 PC . . . .

(X) SUN . . . .

( ) HP . . . .

( ) DEC . . . .

( ) IBM . . . .

( ) . . . .

Operating System

(X) Linux . . . .

(X) Solaris . . . .

( ) HP-UX . . . .

( ) MacOS . . . .

( ) other UNIX . . . .

( ) MS Windows . . . .

( ) . . . .

Compiler

Fortran

- **(X)** g77
- **( )** g90
- **( )** Absoft f77
- **( )** Absoft f90
- **( )** Sun Workshop f77
- **( )** Sun Workshop f90
- **(X)** Intel . . . .
- **( )** . . . .

C/C++

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

( ) other (. . . .)

Memory Requirements (MB): . . . .

Processor Speed (MHz): . . . .

Standard computation time for one model: . . . .

6.11 Remarks

Revising code for more accurate treatment of H_2 . . . .

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Chapter 7

KOSMA-tau

7.1 Model Identification

Name: KOSMA-tau . . . .

List of Authors: A. Sternberg, J. Stutzki, Herbert Störzer, Benedikt Köster, Maik Zilinsky, Uwe Leuenhagen, Solei Jeyakumar . . . .

Institute: KOSMA, I.Physikalisches Institut, Universität zu Köln . . . .

Tel Aviv University (tau), Ramat Aviv 69978, Israel . . . .

Contact Email: roellig@ph1.uni-koeln.de . . . .

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

Störzer, Stutzki & Sternberg, A& A 310, 592 (1996) . . . .

Köster (PhD Thesis, U Köln), Köster et al. A&A 284, 545 (1994) . . . .

Zilinsky (PhD Thesis, U Köln), Zilinsky, Störzer & Stutzki, A&A, 358, 723 (2000) . . . .

Jeyakumar & Stutzki (Proceedings SFChem 2002, NRC press, in press) . . . .

Additional Info . . . .

7.2 Geometry

(X) spherical

( ) plane-parallel (semi-infinite)

( ) plane-parallel (finite)

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

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

Density

- **(X)** homogeneous
- **(X)** density gradient (Eq.: $n \propto r^{-\alpha}$ $\alpha \geq 0$ ....)
- **( )** velocity field (Eq.: ....)
- **( )** time dependant geometry (....)

7.3 Radiation Field

(X) isotropic[1] (Ref.:..)

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

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

7.3.1 Radiation sources

(X) external source

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

( ) internal source

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

[1]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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain $\bar{I}_\nu$.

7.4 Chemistry

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

(X) stationary solution(Ref.: Störzer, Stutzki & Sternberg (1996), based on Sternberg & Dalgarno (1995))

Underlying Database

(X) UMIST95 (modified + extended by ^{13}C, and ^{18}O)
( ) UMIST99
( ) NSM
(X) other (additional species: ^{13}C, and ^{18}O)

extension of database:

Ref.: Isotopologues: following Maik Zilinsky (master thesis, U Köln) and Köster et al. A&A 284, 545 (1994) . . . .
Ref.: . . . .

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

(X) variable number of included species (arbitrary; code designed to model the main H,C,O bearing species and their isotopologues (gas phase only); current chemical network includes H,He,C,O,S,Si,N,Mg,Fe, ^{13}C; up to 113 species and 59 isotopologues)

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

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

(X) formation of H_2 on grains (Ref./Eq.: Sternberg & Dalgarno ApJS 99, 565 (1995) Eq. (A7)-(A9) . . . .)

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

( ) desorption mechanisms included

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

(X) metallicity effects included

scaling relation heating/cooling, abundance: $n(z) = z * n_{z=0}$ $z = 1 =$solar.

(X) scaling law[2] for elemental abundances (Eq./Ref.: $n(z) = z * n_{z=0}$ ....)
(X) scaling law[3] for dust abundance (Eq./Ref.: $n_d(z) = z * n_{d,z=0}$ ....)
(X) scaling law[3] for PAH abundance (Eq./Ref.: $n(z) = z * n_{z=0}$ ....)
(X) metallicity dependant heating rates (Ref.: $\Gamma(z) = z * \Gamma(z=0)$ ....)
(X) metallicity dependant cooling rates (Ref.:$\Lambda(z) = z * \Lambda(z=0)$ ....)

(X) isotoplogues included

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

( ) other ....

( ) other ....

7.5 Thermal Balance

(X) fixed temperature law (Eq.: T_{gas} =const. ....)

(X) temperature determined from energy balance

Cooling Functions

(X) gas-grain heating or cooling (Ref.: Tielens & Hollenbach, ApJ 1985 291, 722 ....)
(X) radiative line cooling (details in section 13.6.2)
(X) recombination cooling (Bakes & Tielens, ApJ 427, 822 (1994) Eq. 4) ....
( ) ....

Heating Functions

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

(X) H_2^* vibrational deexcitation

- **( )** single line approximation(Ref.: . . . .)
- **(X)** only ν-levels but no J(ground state ν=0-14, Lyman band 24 level + Werner band 10 level . . . .)
- **( )** full rot-vib treatment (number of ν/J levels: . . . .)
  Ref.: . . . .)

(X) H_2 dissociation (Ref.: . . . .)

(X) H_2 formation (Ref.: $\propto \frac{1}{3} E_{binding} R_{form} n_H$ . . . .)

(X) CR heating ($\Lambda_{cr} = 61610 \times \zeta$ (cm^{-1}H-particle^{-1} s^{-1}) with CR destruction rate
$\zeta = 5 \times 10^{-17}$ . . . .)

(X) PE heating (Ref.: Bakes & Tielens, 1994, ApJ, 427, 822 . . . .)

( ) XR heating (Ref.: . . . .)

( ) PAH heating (Ref.: . . . .)

( ) . . . .

( ) . . . .

7.6 Radiative Transfer

7.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(X) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

(X) via simple exponentials (Ref.: . . . .
. . . .)

( ) via biexponentials (e.g. Sternberg & Dalgarno 1995) (Ref.: . . . .
. . . .)

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

Dust Properties

(X) treatment of radiative transfer (Ref.: Hollenbach, Takahashi & Tielens, ApJ, 377, 192 (1991))

(X) grain size distribution (PAHs as chemical species: MRN size distribution for $30 \leq N_C \leq 1500$. For photoelectric heating: see Bakes & Tielens, 1994, ApJ, 427, 822)

(X) extinction/scattering law in UV(normalized to A_V(Ref.: $\propto exp\left(-k_\nu \frac{\tau_{UV}}{4}\right)$)

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

(X) scattering function (Eq./Ref.:pure forward scattering . . . .)

Shielding of H_2

( ) No

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

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

(X) detailed solution (Ref.: Störzer et al. 1996 . . . .)

Shielding of CO

( ) No

(X) shielding factors (Ref.: van Dishoeck & Black, ApJ 334, 771 (1988) . . . .)

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

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

(X) Isotope selective photodissociation(Ref.: van Dishoeck & Black, ApJ 334, 771 (1988) . . . .)

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

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

( ) Voigt

( ) Box (width: . . . .)

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

7.6.2 Radiative Transfer in Cooling Lines

Method:

(X) Escape probability (Ref.: Störzer, Stutzki & Sternberg, A&A 310, 592 (1996) . . . .

$\beta(\vec{r}) =$ . . . .)

( ) other . . . .

( ) Solution of RT equation in given geometry

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

Remarks . . . .)

Cooling Lines included:

(X) O (63μ,146μ,44μ. . . . .)

(X) ^{12}CO rotational lines (up to J: 50);

(X) ^{12}C^{+} (158 μ)

(X) ^{12}C (610 μ,370 μ,230μ . . . .)

(X) Si^{+} (35 μ)

(X) ^{13}CO rotational lines (up to J: 50)

(X) OH rotational lines (up to J: 16, 38 transistions and approximation, see Hollenbach & McKee
ApJS, 41, 555 (1979).)

(X) H_2O rotational lines (ortho (lev:31, trans.:92), para (lev:16, trans,:33), and approximation, see
Neufeld & Melnick ApJ 322, 266 (1987))

( ) . . . .

( ) . . . .

7.6.3 Radiative Transfer of Observable Line Intensities

Method:

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

(X) other: ray tracing, ONION, see Gierens, Stutzki & Winnewisser,
A&A 259, 271 (1992) . . . .

( ) no separate treatment from cooling lines (fully self-consistent)

(X) Solution of RT equation in given geometry

Remarks . . . .)

Lines included:

(X) O (no. of lines: 3)

(X) C (no. of lines: 3)

(X) C^{+} (no. of lines: 1)

(X) CO (no. of lines: 50)

(X) ^{13}CO (no. of lines: 50)

(X) C^{18}O (no. of lines: 50)

(X) ^{13}C^{18}O (no. of lines: 50)

( ) H_2O (no. of lines:...........)

( ) $H_2{}^{18}O$ (no. of lines:...........)

(X) other: HCO^+ (no. of lines: 16)(Ref.:. . . . .)
( ) other ....(no. of lines:...........)(Ref.:. . . . .)
( ) other ....(no. of lines:...........)(Ref.:. . . . .)

Computed Line Properties:

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

. . . .)

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

. . . .

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

. . . .)

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

. . . .)

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

. . . .)

Local velocity dispersion/line profile

(X) Gaussian (doppler parameter: β adjusted to the PDR model parameter, including thermal and turbulent component . . . .)
( ) Box (width: . . . .)
( ) other (Ref.:. . . . .)

(X) antenna characteristics included

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

(X) turbulence included: Gaussian line width > thermal line width. . . . .

( ) . . . .

( ) . . . .

7.7 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.: . . . .)
- **(X)** CO-H_2 (Ref.:Schinke et al, 1985, ApJ 299,939 . . . .)
- **(X)** CO-*e* (Ref.:Elitzur, 1977, A&A 57, 179 . . . .)
- **( )** C^+-*e* (Ref.: . . . .)
- **(X)** C^+-H_2 (Ref.:Flower and Launay, 1977, J.Phys. B, 10/5, 879 . . . .)
- **(X)** C^+-H (Ref.:Flower and Launay, 1977, J.Phys. B, 10/5, 879 . . . .)
- **( )** OI-*e* (Ref.: . . . .)
- **( )** OI-H_2 (Ref.: . . . .)
- **( )** OI-H (Ref.: . . . .)
- **( )** C-H (Ref.:Launay and Roueff, 1977, A&A, 56, 289 . . . .)
- **( )** O-H (Ref.:Launay and Roueff, 1977, A&A, 56, 289 . . . .)
- **( )** ...-H (Ref.: . . . .)
- **( )** C-H_2 (Ref.:Spaans et al, 1994,ApJ 437, Schroeder et al,1991, J.Phys. B, 24, 2487, Jaquet et al 1992, J.Phys. B 25, 285 . . . .)
- **( )** O-H_2 (Ref.:see above . . . .)
- **( )** OH-H_2 (Ref.:Dewanger 1987, MNRAS 226, 505 . . . .)
- **( )** He-H_2O (Ref.:Palma et al, 1988 . . . .)
- **( )** ...-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.: . . . .
. . . .)

7.8 Output

PDR code:

(X) abundance profiles over (A_V/depth) . . . .

(X) column density over (A_V/depth) . . . .

(X) temperature profile over (A_V/depth) . . . .

(X) heating and cooling over (A_V/depth) and the contribution by different processes discussed above . . . .

(X) chemical rates over (A_V/depth) . . . .

ONION code:

(X) line integrated intensity (details at 13.6.3) . . . .

(X) line peak temperature . . . .

(X) line profiles . . . .

(X) opacities at linecenters . . . .

( ) . . . .

7.9 Numerics

Gridded variables

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

Gridding strategies: . . . .

Adaptive grid, with an pre-defined upper limit for the total number of shells (typ. $N_{\rm shell} < 400$). . . . .

. . . .

Numerical method to solve the chemical network: rate equations solved using Newton-Raphson method

(Sternberg & Dalgarno, 1995).

. . . .

. . . .

. . . .

(Ref.: Routine DGESV from LAPACK, Numerical Recipes, Press et al. . . . .)

Numerical method to solve the thermal balance: root finding method of Anderson, Bjoerck and King

. . . .

. . . .

. . . .

(Ref.:)

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

In PDR model (in order to calculate the cooling by line emission): escape probability method . . . .

. . . .

(Ref.: Störzer, Stutzki & Sternberg (1996) . . . .)

Description of the iteration schemes . . . .

. . . .

. . . .

. . . .

. . . .

Numerical parameters to tune convergence/computation speed/accuracy

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

Usage of numerical standard routines/packages: code is self-contained; uses subroutines from the Numerical Recipes in F

( ) NAG
(X) BLAS
(X) SLATEC
( ) ODEPACK (LSODE)
( ) LINPACK
(X) Numerical Recipes in Fortran . . . .
( ) . . . .

7.10 Misc

Hardware

- **(X)** x86 PC . . . .
- **(X)** SUN . . . .
- **(X)** HP . . . .
- **( )** DEC . . . .
- **( )** IBM . . . .
- **( )** . . . .

Operating System

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

Compiler

Fortran

- **(X)** g77
- **(X)** g90
- **(X)** Absoft f77
- **( )** Absoft f90
- **(X)** Sun Workshop f77
- **(X)** Sun Workshop f90
- **( )** . . . .
- **( )** . . . .

C/C++

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

( ) other (. . . .)

Memory Requirements (MB): $\approx$ 170 . . . .

Processor Speed (MHz): 2.4 GHz P4 . . . .

Standard computation time for one model: between a few minutes to 1 day, depending on the number of species included and model parameters . . . .

7.11 Remarks

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Chapter 8

Lee96mod

8.1 Model Identification

Name of the Model Lee96mod . . . .

List of Authors H.-H. Lee, E. Herbst, Pineau des Fôrets, E. Roueff, J. Le Bourlot, ...

Institute OSU, Observatoire de Paris . . . .

Contact Email omorata@mps.ohio-state.edu . . . .

Model has been presented/discussed in (Ref.): Lee et al., 1996, A&A 311, 690 . . . .

. . . .

. . . .

Additional Info Chemical network and solverof the network are from the New Standard Model of Eric Herbst. Calculation of CO and H_2 shielding factors is added by Lee et al. (1996) . . . .

. . . .

8.2 Geometry

( ) spherical

(X) plane-parallel (semi-infinite)

( ) plane-parallel (finite)

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

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

Density

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

8.3 Radiation Field

( ) isotropic[1] (Ref.: . . . .)

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

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

8.3.1 Radiation sources

( ) external source

- **( )** Habing field
- **( )** Draine field
- **(X)** Other (Ref.:MMP (Mathis et al., 1983, A&A 128,212 . . . .)
- **( )** detailed spectral energy distribution (Ref.: . . . .)

( ) internal source

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

8.4 Chemistry

(X) time dependant solution(Ref.: Lee et al. (1996) . . . .)

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

Underlying Database

[1]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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain $\bar{I}_\nu$.

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

extension of database:

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

(X) fixed number of included species (number: 419)

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

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

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

(X) 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[2] 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

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

- **( )** ^{18}O
- **( )** ....
- **( )** ....

( ) other ....

( ) other ....

8.5 Thermal Balance

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

( ) temperature determined from energy balance

Cooling Functions

- **( )** gas-grain cooling (Ref.: ....)
- **( )** radiative line cooling (details in section 13.6.2)
- **( )** ....
- **( )** ....

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.: ....)
- **( )** ....
- **( )** ....

8.6 Radiative Transfer

8.6.1 UV transfer

(X) RT solved for precomputed density and temperature structure

( ) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

- **(X)** 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.: . . . .)
- **(X)** extinction/scattering law in UV(normalized to A_V(Ref.: . . . .)
- **( )** albedo (Ref.: . . . .)
- **( )** scattering function (Eq./Ref.: . . . .)

Shielding of H_2

- **( )** No
- **(X)** shielding factors (Ref.: . . . .)
- **( )** single line Ref.: . . . .)
- **( )** detailed solution (Ref.: . . . .)

Shielding of CO

- **( )** No
- **(X)** 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.: . . . .)

8.6.2 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:........)
- **( )** ....
- **( )** ....

8.6.3 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.: . . . .)

( ) . . . .

( ) . . . .

8.7 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.: . . . .
. . . .)

8.8 Output

(X) abundance profiles over (A_V/depth)

( ) temperature profile over (A_V/depth)

( ) emitted intensities (details at 13.6.3)

( ) opacities at linecenters (. . . .)

( ) . . . .

( ) . . . .

( ) . . . .

8.9 Numerics

Gridded variables

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

Gridding strategies: Spatial coordinate is gridded logarithmically at small A_V. At large A_V, it is gridded linearly. Time spacing is automatically calculated so that the temporal variation in the abundance is not too large . . . .

. . . .

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

. . . .

. . . .

(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 (. . . .)
- **(X)** accuracy goal (10^{-4} . . . .)
- **( )** starting solution (. . . .)
- **( )** methods for convergence acceleration (. . . .)
- **( )** parallelized code(. . . .)
- **( )** . . . .
- **( )** . . . .

Usage of numerical standard routines/packages

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

8.10 Misc

Hardware

- **( )** x86 PC ....
- **( )** SUN ....
- **( )** HP ....
- **( )** DEC ....
- **( )** IBM ....
- **(X)** Cray ....

Operating System

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

Compiler

Fortran

- **( )** g77
- **( )** g90
- **( )** Absoft f77
- **( )** Absoft f90
- **( )** Sun Workshop f77
- **( )** Sun Workshop f90
- **(X)** Cray Fortran 90 ....
- **( )** ....

C/C++

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

( ) other (....................)

Memory Requirements (MB): ....

Processor Speed (MHz): ....

Standard computation time for one model: $\sim$ 3h ....

8.11 Remarks

. . . .

. . . .

. . . .

. . . .

. . . .

. . . .

. . . .

. . . .

Chapter 9

Leiden

9.1 Model Identification

Name of the Model cloud/chemism

List of Authors John Black, Ewine van Dishoeck

Institute Leiden Observatory

Contact Email ewine@strw.leidenuniv.nl

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

Black & van Dishoeck ApJ 322 412 1987

additions in Jansen et al. A&A 302 223 1995

Additional Info . . . .

. . . .

. . . .

. . . .

9.2 Geometry

( ) spherical

(X) plane-parallel (semi-infinite)

(X) plane-parallel (finite)

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

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

Density

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

9.3 Radiation Field

( ) isotropic[1] (Ref.: . . . .)

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

(X) other (Ref.: two-sided)

9.3.1 Radiation sources

(X) external source

- **(X)** Habing field
- **(X)** Draine field
- **(X)** Other (Ref.: user input)
- **( )** detailed spectral energy distribution (Ref.: . . . .)

( ) internal source

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

9.4 Chemistry

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

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

Underlying Database

- **(X)** UMIST95
- **( )** UMIST99

[1] 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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain $\bar{I}_\nu$.

( ) NSM
(X) other (Ref.: van Dishoeck & Black ApJS 62 109 1986)

extension of database:

Ref.: Blake et al. ApJ 300 415 1986 (Cl chemistry)
Ref.: Drdla et al. ApJ 345 815 1986 (S chemistry)
Ref.: van Dishoeck, in Rate coefficients in astrochemistry, eds Millar & Williams, (Dordrecht: Kluwer) 49 1988 (photo rates)

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

(X) variable number of included species (44 - 215)

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

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

(X) formation of H_2 on grains (Ref./Eq.:$R_{\rm form} = 3 \times 10^{-18} \sqrt{T} \frac{y_f\, n({\rm H})\, n_{\rm H}}{1+T/T_{\rm form}}$; $T_{\rm form}$=400 K)

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

( ) desorption mechanisms included

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

(X) metallicity effects included

( ) scaling law[2] 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

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

( ) other . . . .

( ) other . . . .

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

9.5 Thermal Balance

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

(X) temperature determined from energy balance

Cooling Functions

- **(X)** gas-grain cooling (Ref.: Burke & Hollenbach AJ 265 223 1983)
- **(X)** radiative line cooling (details in section 13.6.2)
- **( )** . . . .
- **( )** . . . .

Heating Functions

- **(X)** H_2^* vibrational deexcitation
  - **(X)** single line approximation(Ref.: Tielens & Hollenbach ApJ 291 722 1985)
  - **( )** only ν-levels but no J(Ref.: . . . .)
  - **( )** full rot-vib treatment (number of ν/J levels: . . . . Ref.: . . . .)
- **(X)** H_2 dissociation (Ref.: Stephens & Dalgarno Quant. spect. rad. tranf. 12 569 1972)
- **(X)** H_2 formation (Ref.: Jura ApJ 197 575 1975)
- **(X)** CR heating (Ref.: $\Gamma_{CR} = \zeta_{CR}\,(2.5\times10^{-11}\,n(H_2)+5.5\times10^{-12}\,n(H))\,\mathrm{erg\,s^{-1}\,cm^{-3}}$)
- **(X)** PE heating (Ref.:de Jong A&A 55 137 1977)
- **( )** XR heating (Ref.: . . . .)
- **(X)** PAH heating (Ref.: Bakes & Tielens ApJ 427 822 1994, $30 < N_C < 530$)
- **(X)** C ionization, $\sigma_{ion} = 10^{-17}\,\mathrm{cm^2}$ for $h\nu > 11$ eV
- **(X)** Chemical heating

9.6 Radiative Transfer

9.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(X) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

- **(X)** via simple exponentials (e.g. like in UMIST) (Ref.: . . . .)

( ) via biexponentials (e.g. Sternberg & Dalgarno 1995) (Ref.: ....
....)

(X) other (Ref.: explicit calculation using grain properties)

Dust Properties

(X) treatment of radiative transfer (Ref.: Roberge et al. ApJS 77 287 1991)

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

(X) extinction/scattering law in UV(normalized to A_V(Ref.:Roberge et al. 1991)

(X) albedo (Ref.: Roberge et al 1991)

(X) scattering function (Eq./Ref.: Roberge et al 1991)

Shielding of H_2

( ) No

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

( ) single line Ref.:...)

(X) detailed solution (Ref.: Black & van Dishoeck 1987)

Shielding of CO

( ) No

(X) shielding factors (Ref.: van Dishoeck & Black ApJ 334 771 1988)

(X) single line (Ref.: van Dishoeck & Black 1988)

(X) detailed solution (Ref.: van Dishoeck & Black 1988)

(X) Isotope selective photodissociation(Ref.: van Dishoeck & Black 1988)

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

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

(X) Voigt

( ) Box (width: ....)

( ) other (Ref.:..)

9.6.2 Radiative Transfer in Cooling Lines

Method:

(X) Escape probability (Ref.: ....
$\beta(\vec{r}) = 0.5\,(1 - e^{-3\tau})/3\tau)$

( ) other ....

( ) Solution of RT equation in given geometry

(X) IR pumping (e.g. OI) (Ref.: Hollenbach et al ApJ 377 192 1991)

Remarks . . . .)

Cooling Lines included:

- **(X)** O (63μ,146μ, ...)
- **(X)** ^{12}CO rotational lines (up to J: 20)
- **(X)** $^{12}C^+$ (158 μ)
- **(X)** ^{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:........)
- **( )** . . . .
- **( )** . . . .

9.6.3 Radiative Transfer of Observable Line Intensities

Method:

- **(X)** Escape probability (Ref.: . . . .
  $\beta(\vec{r}) = (1 - e^{-3\tau})/3\tau$)
- **( )** other . . . .
- **( )** no separate treatment from cooling lines (fully self-consistent)

( ) Solution of RT equation in given geometry

Remarks . . . .)

Lines included:

- **(X)** O (no. of lines: 2)
- **(X)** C (no. of lines: 2)
- **(X)** C^+ (no. of lines: 1)
- **( )** 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.: . . . .)

Computed Line Properties:

(X) fully resolved line profiles (remark: full ratiative transfer of observable lines can be done in a separate Monte-Carlo radiative transfer package)

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

. . . .

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

. . . .)

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

. . . .)

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

. . . .)

Local velocity dispersion/line profile

- **(X)** Gaussian (doppler parameter: variable (2 km/s default))
- **( )** Box (width: . . . .)
- **( )** other (Ref.: . . . .)

( ) antenna characteristics included

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

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

( ) . . . .

( ) . . . .

9.7 Rate Coefficients

Collision Rates

- **( )** H-H (Ref.: . . . .)
- **(X)** H-H_2(Ref.: . . . .)
- **( )** H_2-H^+ (Ref.: . . . .)
- **( )** H_2-*e* (Ref.: . . . .)
- **(X)** H_2-H_2 (Ref.: . . . .)
- **(X)** CO-H (Ref.: Warin et al. A&A 308 535 1996)
- **(X)** CO-H_2 (Ref.: Flower J. Phys. B 34 1 2001)
- **( )** CO-*e* (Ref.: . . . .)
- **(X)** C^+-*e* (Ref.: Black fit to Hayes & Nussbaumer A&A 134 193 1984)
- **(X)** C^+-H_2 (Ref.: Black fit to Flower & Launay J. Phys. B 10 3673 1977)
- **(X)** C^+-H (Ref.: Black fit to Launay & Roueff J. Phys. B 10 879 1977)
- **(X)** OI-*e* (Ref.: Liseau fit to Bell et al. MNRAS 293 L83 1998)
- **(X)** OI-H_2 (Ref.: Li fit to Jaquet et al. J. Phys. B 25 285 1992)
- **(X)** OI-H (Ref.: Liseau fit to Launay & Roueff 1977)
- **(X)** C-H (Ref.: Launay & Roueff 1977)
- **( )** ...-H (Ref.: . . . .)
- **( )** ...-H (Ref.: . . . .)
- **(X)** C-H_2 (Ref.: Schröder et al. J. Phys. B 24 2487 1991)
- **( )** ...-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

(X) CO (Ref.: Kamp & van Zadelhoff A&A 373 641 2001
. . . .)

(X) H_2 (Ref.: Turner et al. ApJS 35 281 1977
. . . .)

(X) C (Ref.: Nussbaumer & Rusca A&A 72 129 1979
. . . .)

(X) O (Ref.: Mendoza in IAU symposium 103: Planetary nebulae, ed. D.R. Flower (Dordrecht: Reidel) 143 1983)

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

(X) C^+ (Ref.: Nussbaumer & Storey A&A 96 91 1981
. . . .)

( ) H_2O (Ref.: . . . .
. . . .)

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

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

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

9.8 Output

(X) abundance profiles over (A_V/depth)

(X) temperature profile over (A_V/depth)

(X) emitted intensities (details at 13.6.3)

(X) opacities at linecenters (. . . .)

( ) . . . .

( ) . . . .

( ) . . . .

9.9 Numerics

Gridded variables

- **(X)** frequency/wavelength
- **( )** temperature
- **(X)** spatial coordinate(s)
- **( )** velocity
- **( )** time
- **(X)** H_2 column
- **( )** ....

Gridding strategies: Fine sampling of H-H_2 transition in region where N(H_2)=10^{13} – 10^{19} cm^{-2}

....

Numerical method to solve the chemical network: LU decomposition

....

....

(Ref.: Numerical recipes)

Numerical method to solve the thermal balance: Brent's method

....

....

(Ref.: Numerical recipes)

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

continuum: spherical harmonics

lines: van Dishoeck & Black 1988

(Ref.: Roberge et al. 1991)

Description of the iteration schemes ....

See above numerical methods

For 2-sided models there is an iteration on H_2 and CO column densities

....

....

Numerical parameters to tune convergence/computation speed/accuracy

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

Usage of numerical standard routines/packages

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

9.10 Misc

Hardware

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

Operating System

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

Compiler

Fortran

- **(X)** g77
- **( )** g90
- **( )** Absoft f77
- **( )** Absoft f90
- **( )** Sun Workshop f77
- **( )** Sun Workshop f90
- **( )** ....
- **( )** ....

C/C++

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

( ) other (....)

Memory Requirements (MB): $<$ 512 MB

Processor Speed (MHz): 500 MHz

Standard computation time for one model:

fast CO dissociation, no temperature iteration: 2 minutes

full H_2, CO dissociation, thermal balance: 20 minutes

9.11 Remarks

....

....

....

....

....

....

Chapter 10

Meijerink

10.1 Model Identification

Combined PDR and XDR code . . . .

Rowin Meijerink, Marco Spaans . . . .

Leiden Observatory, Kapteyn Institute . . . .

meijerin@strw.leidenuniv.nl, spaans@astro.rug.nl . . . .

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

. . . .

. . . .

Additional Info . . . .

. . . .

. . . .

. . . .

10.2 Geometry

( ) spherical

(X) plane-parallel (semi-infinite)

( ) plane-parallel (finite)

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

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

Density

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

10.3 Radiation Field

( ) isotropic[1] (Ref.: . . . .)

(X) uni-directional (Ref.: Tielens & Hollenbach 1985 . . . .)

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

10.3.1 Radiation sources

(X) external source

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

( ) internal source

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

10.4 Chemistry

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

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

Underlying Database

- **(X)** UMIST95
- **( )** UMIST99

[1]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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain I_ν.

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

extension of database:

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

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

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

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

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

(X) formation of H_2 on grains (Ref./Eq.: Cazaux et al. 2003 . . . .)

( ) 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[2] 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 . . . .

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

10.5 Thermal Balance

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

(X) temperature determined from energy balance

Cooling Functions

- **(X)** gas-grain cooling (Ref.: Tielens & Hollenbach 1985 . . . .)
- **(X)** radiative line cooling (details in section 13.6.2)
- **( )** . . . .
- **( )** . . . .

Heating Functions

- **(X)** H_2^* vibrational deexcitation
  - **(X)** single line approximation(Ref.: Tielens & Hollenbach 1985 . . . .)
  - **( )** only ν-levels but no J(Ref.: . . . .)
  - **( )** full rot-vib treatment (number of ν/J levels: . . . .
    Ref.: . . . .)
- **(X)** H_2 dissociation (Ref.: Tielens & Hollenbach 1985 . . . .)
- **( )** H_2 formation (Ref.: . . . .)
- **(X)** CR heating (Ref.: Tielens & Hollenbach 1985 . . . .)
- **( )** PE heating (Ref.: . . . .)
- **( )** XR heating (Ref.: . . . .)
- **(X)** PAH heating (Ref.: Bakes & Tielens 1994 . . . .)
- **( )** . . . .
- **( )** . . . .

10.6 Radiative Transfer

10.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(X) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

- **(X)** 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.: . . . .)

(X) single line Ref.: Tielens & Hollenbach 1985 . . . .)

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

Shielding of CO

( ) No

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

(X) single line Ref.: Tielens & Hollenbach 1985 . . . .)

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

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

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

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

( ) Voigt

( ) Box (width: . . . .)

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

10.6.2 Radiative Transfer in Cooling Lines

Method:

(X) Escape probability (Ref.: Tielens & Hollenbach 1985 . . . .
$\beta(\vec{r}) =$ . . . .)

( ) other . . . .

( ) Solution of RT equation in given geometry

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

Remarks . . . .)

Cooling Lines included:

- **(X)** O (63μ,146μ, ...)
- **(X)** ^{12}CO rotational lines (up to J: 26)
- **(X)** $^{12}C^+$ (158 μ)
- **(X)** ^{12}C (610 μ,370 μ, ...)
- **(X)** Si^+ (35 μ)
- **(X)** ^{13}CO rotational lines (up to J: 26)
- **(X)** OH rotational lines (up to J: 36)
- **(X)** H_2O rotational lines (up to J:45)
- **( )** . . . .
- **( )** . . . .

10.6.3 Radiative Transfer of Observable Line Intensities

Method:

- **(X)** Escape probability (Ref.: Tielens & Hollenbach 1985 . . . .
  $\beta(\vec{r}) =$ . . . .)
- **( )** other . . . .
- **( )** no separate treatment from cooling lines (fully self-consistent)

( ) Solution of RT equation in given geometry

Remarks . . . .)

Lines included:

- **(X)** O (no. of lines:3 finestructure lines)
- **(X)** C (no. of lines:3 finestructure lines)
- **(X)** C^+ (no. of lines:1 finestructe line)
- **( )** 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: . . . .

. . . .)

(X) 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.: . . . .)

( ) . . . .

( ) . . . .

10.7 Rate Coefficients

Collision Rates

- **( )** H-H (Ref.: . . . .)
- **( )** H-H_2(Ref.: . . . .)
- **( )** H_2-H^+ (Ref.: . . . .)
- **( )** H_2-*e* (Ref.: . . . .)
- **( )** H_2-H_2 (Ref.: . . . .)
- **(X)** CO-H (Ref.: Chu and Dalgarno . . . .)
- **(X)** CO-H_2 (Ref.: Schinke et al. 1985 . . . .)
- **(X)** CO-*e* (Ref.: eimpact program . . . .)
- **( )** C^+-*e* (Ref.: . . . .)
- **(X)** C^+-H_2 (Ref.: Spaans et al. 1994 . . . .)
- **( )** C^+-H (Ref.: . . . .)
- **( )** OI-*e* (Ref.: . . . .)
- **(X)** OI-H_2 (Ref.: Spaans et al. 1994 . . . .)
- **( )** 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

(X) CO (Ref.: Ewine database . . . .)

(X) H_2 (Ref.: Ewine database . . . .)

(X) C (Ref.: Tielens & Hollenbach 1985 . . . .)

(X) O (Ref.: Tielens & Hollenbach 1985 . . . .)

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

(X) C^+ (Ref.: Tielens & Hollenbach 1995 . . . .)

( ) H_2O (Ref.: . . . .)

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

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

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

10.8 Output

(X) abundance profiles over (A_V/depth)

(X) temperature profile over (A_V/depth)

(X) emitted intensities (details at 13.6.3)

( ) opacities at linecenters (. . . .)

( ) . . . .

( ) . . . .

( ) . . . .

10.9 Numerics

Gridded variables

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

Gridding strategies: . . . .

. . . .

. . . .

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

LU docomposition . . . .

. . . .

(Ref.: Numerical recipies . . . .)

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

Bisection method . . . .

. . . .

(Ref.: . . . .)

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

Excape probabily method . . . .

. . . .

(Ref.: . . . .)

Description of the iteration schemes . . . .

chemical balance (T, 0.5 * T and 2.0 * T), thermal balance (T, 0.5 * T, 2.0 * T) . .

bisection till convertion. . . . .

. . . .

. . . .

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
- **( )** . . . .
- **( )** . . . .

10.10 Misc

Hardware

- **(X)** x86 PC . . . .
- **( )** SUN . . . .
- **( )** HP . . . .
- **( )** DEC . . . .
- **( )** IBM . . . .
- **( )** . . . .

Operating System

- **(X)** 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++

- **(X)** gcc
- **( )** Sun Workshop C/C++ compiler
- **( )** ....
- **( )** ....

( ) other (....)

Memory Requirements (MB): $<$ 20 MB ....

Processor Speed (MHz): 2 GHz ....

Standard computation time for one model: few minutes most ....

10.11 Remarks

....

....

....

....

....

....

....

....

Chapter 11

Meudon

11.1 Model Identification

PDR . . . .

Le Bourlot J., Roueff E., Le Petit F. . . . .

LUTH, Observatoire de Paris/Meudon . . . .

jacques.lebourlot@obspm.fr . . . .

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

Le Petit F.,Roueff E. and Le Bourlot J., ”D/HD transition in Photon Dominated Regions (PDR)”, A&A 390, 369-381 (2002) . . . .

Le Bourlot J., ”Ortho to para conversion of H_2 on interstellar grains”, A&A 360, 656-662 (2000) . . . .

Le Bourlot, J. and Pineau Des Forets, G. and Roueff, E. and Flower, D. R., ”Infrared and submillimetric emission lines from the envelopes of dark clouds”, A&A 267, 233-254 (1993) . . . .

Abgrall, H. and Le Bourlot, J. and Pineau Des Forets, G. and Roueff, E. and Flower, D. R. and Heck, L., ”Photodissociation of H2 and the H/H2 transition in interstellar clouds”, A&A 253, 525- (1992) . . . .

Source code, documentation and examples available at: . . . .

http://aristote.obspm.fr/MIS/pdr/pdr1.html . . . .

Published under the GPL . . . .

11.2 Geometry

( ) spherical

(X) plane-parallel (semi-infinite)

(X) plane-parallel (finite)

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

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

Density

- **(X)** homogeneous
- **(X)** density gradient (Eq.: any: analytical or interpolated from file . . . .)
- **( )** velocity field (Eq.: . . . .)
- **( )** time dependant geometry (. . . .)

11.3 Radiation Field

(X) isotropic[1] (Ref.: . . . .)

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

(X) other: Combination of isotropic + illuminating star in vicinity (Ref.:. . . . .)

11.3.1 Radiation sources

(X) external source

- **( )** Habing field
- **(X)** Draine field
- **(X)** Other: Optional star (T_{eff}, R and d) (Ref.: . . . .)
- **(X)** Detailed spectral energy distribution (optional, needs editing a few lines of code)(Ref.: . . . .)

( ) internal source

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

[1] 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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain $\bar{I_\nu}$.

11.4 Chemistry

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

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

Underlying Database

- **(X)** UMIST95
- **( )** UMIST99
- **(X)** NSM
- **(X)** Other (various files in line) Le Bourlot, J. and Pineau Des Forets, G. and Roueff, E. and Flower, D. R., "Infrared and submillimetric emission lines from the envelopes of dark clouds", A&A 267, 233-254(1993) . . . .

extension of database:

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

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

(X) variable number of included species (....30.....-...450...)

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

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

(X) formation of H_2 on grains (Ref./Eq.: Le Bourlot, J., "Ortho to para conversion of H_2 on interstellar grains", A&A 360, 656-662 (2000) . . . .)

(X) formation of other molecules on grains (Ref./Eq.: HD in Le Petit et al, 2002 . .)

(X) desorption mechanisms included

- **(X)** photoevaporation
- **(X)** CR spot heating
- **(X)** grain-grain collisions ref : Le Bourlot, J. and Pineau des Forets, G. and Roueff, E. and Flower, D. R., "On the uniqueness of the solutions to the chemical rate equations in inter stellar clouds: the gas-dust interface.", A &A 302, 870 (1995)
- **( )** grain sputtering

(X) metallicity effects included

- **( )** scaling law[2] for elemental abundances (Eq./Ref.: . . . .)

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

- **( )** 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

- **(X)** D
- **(X)** ^{13}C
- **( )** ^{17}O
- **(X)** ^{18}O
- **( )** Optionally expandable . . . .
- **( )** . . . .

( ) other . . . .

( ) other . . . .

11.5 Thermal Balance

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

(X) temperature determined from energy balance

Cooling Functions

- **(X)** Gas-grain cooling (Ref.: Le Bourlot, J. and Pineau des Forets, G. and Roueff, E. and Flower, D. R., "On the uniqueness of the solutions to the chemical rate equations in interstellar clouds: the gas-dust interface.", A &A 302, 870 (1995) . . . .)
- **(X)** Radiative line cooling (details in section 13.6.2)
- **(X)** Chemical balance . . . .
- **( )** . . . .

Heating Functions

- **(X)** H_2^* vibrational deexcitation
  - **( )** single line approximation(Ref.: . . . .)
  - **( )** only ν-levels but no J(Ref.: . . . .)
  - **(X)** full rot-vib treatment (number of ν/J levels:Optional, up to all . . . . . . Ref.: . . . .)
- **(X)** H_2 dissociation (Ref.: Abgrall et al. 1992, Abgrall H., Roueff E., Drira I., "Total transition probability and spontaneous radiative dissociation of B, C, B' and D states of molecular hydrogen" A &A S 141, 297 (2000) . . . .)

(X) H_2 formation (Ref.: Le Petit et al. 2002, ...)
(X) CR heating (Ref.: . . . .)
(X) PE heating (Ref.: . . . .)
( ) XR heating (Ref.: . . . .)
(X) PAH heating (Ref.: . . . .)
(X) Chemical balance . . . .
( ) . . . .

11.6 Radiative Transfer

11.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(X) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

(X except H2, HD, CO, C, S) via simple exponentials (e.g. like in UMIST) (Ref.: . . . .
( ) via biexponentials (e.g. Sternberg & Dalgarno 1995) (Ref.: . . . .
. . . .)
(X) other: H2, HD, CO, C, S: full RT in lines (Ref.: . . . .)

Dust Properties

(X) treatment of radiative transfer (Ref.: . . . .)
(X) grain size distribution (Ref.: MRN . . . .)
(X) extinction/scattering law in UV(normalized to A_V)(Ref.: Fitzpatrick & Massa 1990 . . . .)
(X) albedo (Ref.: Mathis 1996 . . . .)
(X) scattering function (Eq./Ref.: Weingartner & Draine 2001 . . . .)

Shielding of H_2

( ) No
( ) shielding factors (Ref.: . . . .)
( ) single line Ref.: . . . .)
(X) detailed solutions (exact for lowest levels, FGK approximation above) (Ref.:)

Shielding of CO

( ) No
( ) shielding factors (Ref.: . . . .)
( ) single line Ref.: . . . .)
(X) detailed solution (Ref.: . . . .)
(X) Isotope selective photodissociation(Ref.: . . . .)

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

( ) Gaussian (doppler parameter: . . . .)
(X) Voigt
( ) Box (width: . . . .)
( ) other (Ref.: . . . .)

11.6.2 Radiative Transfer in Cooling Lines

Method:

(X) Escape probability (Ref.: de Jong, Boland, Dalgarno (1980) . . . .
$\beta(\vec{r}) =$ . . . .)
( ) other . . . .

( ) Solution of RT equation in given geometry

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

Remarks Chemical formation and destruction included in detailed balance . . . .

Cooling Lines included:

(X) H_2 (rotational and rovibrational . . . .)
(X) HD (rotational . . . .)
(X) O (63μ, 146μ and optical lines . . . .)
(X) ^{12}CO rotational lines (up to J: 30)
(X) $^{12}C^+$ (158 μ)
(X) ^{12}C (610 μ, 370 μ, ...)
(X) Si^+ (35 μ)
(X) ^{13}CO rotational lines (up to J: 30....)
( ) OH rotational lines (up to J:........)
( ) H_2O rotational lines (up to J:........)
(OH & H2O) approximate formula . . . .
(X) full excitation of C, N, O, S, Si and first ion computed . . . .

11.6.3 Radiative Transfer of Observable Line Intensities

Method:

( ) Escape probability (Ref.: . . . .
$\beta(\vec{r}) =$ . . . .)
( ) other . . . .
( ) no separate treatment from cooling lines (fully self-consistent)
(X) Solution of RT equation in given geometry

Remarks: user defined inclination . . . .)

Lines included:

(X) H_2 (rotational and rovibrational . . . .)
(X) HD (rotational . . . .)
(X) O (no. of lines: 5)
(X) C (no. of lines: 5)
(X) C^+ (no. of lines: 3)
(X) CO (no. of lines: 30)
(X) ^{13}CO (no. of lines: 30)
(X) $C^{18}O$ (no. of lines: 30)
(X) $^{13}C^{18}O$ (no. of lines:...........)
( ) H_2O (no. of lines:)
( ) $H_2{}^{18}O$ (no. of lines:...........)
(X) Si^+............(no. of lines:...........)(Ref.: . . . .)
(X) HCO^+........(no. of lines:...........)(Ref.: . . . .)
(X) CS............(no. of lines:...........)(Ref.:. . . . .)

Computed Line Properties:

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

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

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

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

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

(X) Absorption spectrum in U.V. (remark: . . . .

Including lines of H_2 only for now. . . . .)

Local velocity dispersion/line profile

- **(X)** Gaussian (doppler parameter: thermal + turbulent . . . .)
- **( )** Box (width: . . . .)
- **( )** other (Ref.: . . . .)

( ) antenna characteristics included

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

(X) turbulence included: only line broadening (Ref.: . . . .)

( ) . . . .

( ) . . . .

11.7 Rate Coefficients

Collision Rates

- **( )** H-H (Ref.: . . . .)
- **(X)** H-H_2 (described in Ref.: Le Bourlot, J. and Pineau des Forêts, G. and Flower, D. R. , ”The cooling of astrophysical media by H_2”, MNRAS 305, 802-810 (1999) . . . .)
- **( )** H_2-H^+ (Ref.: previous reference . . . .)
- **( )** H_2-e (Ref.: . . . .)
- **( )** H_2-H_2 (Ref.:previous reference . . . .)
- **( )** CO-H (Ref.: Balakrishnan, N. and Yan, M. and Dalgarno, A., ”Quantum-Mechanical Study of Rotational and Vibrational Transitions in CO Induced by H Atoms”, ApJ 568, 443-447 (2002) . . . .)
- **( )** CO-He (Ref.: Cecchi-Pestellini, C. and Bodo, E. and Balakrishnan, N. and Dalgarno, A., ”Rotational and Vibrational Excitation of CO Molecules by Collisions with He Atoms”, ApJ 571, 1015-1020 (2002)) item[( )] CO-H_2 (Ref.: D.R. Flower (2001, J.Phys.B., 34, 2731) . . . .)
- **( )** CO-e (Ref.: . . . .)
- **( )** C^+-e (Ref.: . . . .)
- **( )** C^+-H_2 (Ref.: Flower D.R., Launay J.M., J. PHys. B 10, 3673 (1977) . . . . .)

- **( )** C^+-H (Ref.: Launay J.M., Roueff E., J. Phys. B. 10, 879 (1977) . . . .)
- **( )** OI-*e* (Ref.: . . . .)
- **( )** OI-H_2 (Ref.: Jacquet R., Staemmler V. Smith M.D., Flower D.R. J. Phys. B 25, 285 (1992) . . . .)
- **( )** OI-H (Ref.: Launay J.M., Roueff E., A &A 56, 289 (1977) . . . .)
- **( )** Si^+...-H (Ref.: Roueff 234, 567 (1990) . . . .)
- **( )** HD...-H (Ref.: given in Flower D.R., Le Bourlot J., Pineau des Forêts G., Roueff E., MNRAS 314, 753 (2000) . . . .)
- **( )** HD...-H_2 (Ref.: previous reference . . . .)
- **( )** ...-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.: . . . .)

11.8 Output

(X) abundance profiles over (A_V/depth)

(X) temperature profile over (A_V/depth)

(X) emitted intensities (details at 13.6.3)

(X) opacities at linecenters (. . . . .)

(X) column density . . . .

(X) cooling and heating processes . . . .

(X) chemical rates over (A_V/depth) . . . .

(X) Excitation diagram of H_2 . . . .

11.9 Numerics

Gridded variables

- **(X)** frequency/wavelength
- **( )** temperature
- **(X)** spatial coordinate(s)
- **( )** velocity
- **( )** time
- **remark:** All physical variables are continuous functions of A_v. . . . .

Gridding strategies: . . . .

wavelength: uneven steps, computed once at the begining of a run . . . .

Spatial grid: adaptative logarithmic step size (in A_v) . . . .

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

Newton-Raphson for given T and chemical rates, embedded within an iterative scheme to enforce self-consistency . . . .

(Ref.: . . . .)

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

Adaptative secant . . . .

Abondances and temperature are solved sequencially and iterations are done until consistency is achieved. . . . .

(Ref.: . . . .)

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

Spherical harmonics development of specific intensity . . . .

grains + lines extinction included simultaneously . . . .

(Ref.: expanded from Roberge . . . .)

Description of the iteration schemes Two embedded iterations: . . . .

1 Radiative transfer in whole cloud with previous abundances . . . .

2 Scan through cloud from $A_v = 0$ to A_v^{max} . . . .

3 At each A_v compute: a) chemical rates, b) abundances, c) populations and temperature . . . .

convergence criteria based on various relative variations. . . . .

Numerical parameters to tune convergence/computation speed/accuracy

- **(X)** step size (. . . .)
- **(X)** accuracy goal (. . . .)
- **( )** starting solution (. . . .)
- **(X)** methods for convergence acceleration (. . . .)
- **(.)** parallelized code: work in progress (. . . .)
- **( )** . . . .

Usage of numerical standard routines/packages

- **( )** NAG
- **(X)** BLAS
- **( )** SLATEC
- **( )** ODEPACK (LSODE)
- **( )** LINPACK
- **(X)** LAPACK
- **( )** . . . .

11.10 Misc

Hardware

- **(X)** x86 PC . . . .
- **( )** SUN (not tested) . . . .
- **( )** HP (not tested) . . . .

(X) DEC . . . .
(X) IBM . . . .
( ) . . . .

Operating System

(X) Linux . . . .
( ) Solaris (not tested) . . . .
( ) HP-UX (not tested) . . . .
( ) MacOS (not tested) . . . .
(X) other UNIX . . . .
(X) MS Windows . . . .
(X) Should run on any system with standard Fortran 90 and LAPACK . . . .

Compiler

Fortran

( ) g77
( ) g90
( ) Absoft f77
(X) Absoft f90
( ) Sun Workshop f77
(X) Sun Workshop f90
(X) Portland Group f90 . . . .
(X) Intel ifc . . . .
(X) Microsoft Visual Fortran 90 . . . .

C/C++

(X) gcc (used for one minor optional feature on UNIX systems)
( ) Sun Workshop C/C++ compiler
( ) . . . .
( ) . . . .

( ) other (. . . .)

Memory Requirements (MB): Compiler dependant. about 120 Mb for a standard case . . . .

Processor Speed (MHz): at least 1 Ghz recommanded . . . .

Standard computation time for one model: Anything from 30 mn to 1 day. 2 hours typical . . . .

11.11 Remarks

The code includes developements over 15 years (with oldest parts in f77 and newest in f90). The stress in on micro-physical processes, with as few empirical fits to observational data as possible. . . . .

A paper giving much more details is in preparation, and should be available soon. . .

. . . .

Chapter 12

Sternberg

12.1 Model Identification

Name: SDPDR . . . .

List of Authors: Amiel Sternberg, Alex Dalgarno . . . .

Institute: Tel Aviv University . . . .

Contact Email: amiel@wise.tau.ac.il . . . .

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

Sternberg & Dalgarno, ApJSS, 99, 565-607, 1995 . . . .

Sternberg &Neufeld, ApJ, 516, 371-380, 1999 . . . .

Additional Info . . . .

12.2 Geometry

( ) spherical

(X) plane-parallel (semi-infinite)

( ) plane-parallel (finite)

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

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

Density

(X) homogeneous
(X) density gradient (Eq.: $n \propto r^{-\alpha}$ $\alpha \geq 0$ . . . .)
( ) velocity field (Eq.: . . . .)
( ) time dependant geometry (. . . .)

12.3 Radiation Field

( ) isotropic[1] (Ref.: . . . .)

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

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

12.3.1 Radiation sources

(X) external source

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

( ) internal source

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

12.4 Chemistry

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

(X) stationary solution(Ref.: Sternberg & Dalgarno (1995))

Underlying Database

- **(X)** UMIST95
- **(X)** UMIST99
- **( )** NSM
- **(X)** other (individual special cases)

extension of database:

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

[1] 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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain $\bar{I}_\nu$.

(X) fixed number of included species (number: 78) (H,He,C,O,S,Si,N)

( ) variable number of included species

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

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

(X) formation of H_2 on grains (Ref./Eq.: Sternberg & Dalgarno ApJS 99, 565 (1995) Eq. (A7)-(A9) . . . .)

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

( ) desorption mechanisms included

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

(X) metallicity effects included

scaling relation heating/cooling, abundance: $n(z) = z * n_{z=0}$ $z = 1 =$solar.

- **(X)** scaling law[2] for elemental abundances (Eq./Ref.: $n(z) = z * n_{z=0}$ . . . .)
- **(X)** scaling law[3] for dust abundance (Eq./Ref.: $n_d(z) = z * n_{d,z=0}$ . . . .)
- **( )** scaling law[3] for PAH abundance (Eq./Ref.: . . . .)
- **(X)** metallicity dependant heating rates (Ref.: $\Gamma(z) = z * \Gamma(z = 0)$ . . . .)
- **(X)** metallicity dependant cooling rates (Ref.:$\Lambda(z) = z * \Lambda(z = 0)$ . . . .)

(X) isotoplogues included

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

( ) other . . . .

( ) other . . . .

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

12.5 Thermal Balance

(X) fixed temperature law (Eq.: T_{gas} =const. . . . .)

(X) temperature determined from energy balance

Cooling Functions

- **(X)** gas-grain heating or cooling (Ref.: Tielens & Hollenbach, ApJ 1985 291, 722 . . . .)
- **(X)** radiative line cooling (details in section 13.6.2)
- **(X)** recombination cooling (Bakes & Tielens, ApJ 427, 822 (1994) Eq. 4) . . . .
- **( )** . . . .

Heating Functions

- **(X)** H_2^* vibrational deexcitation
  - **( )** single line approximation(Ref.: . . . .)
  - **(X)** only ν-levels but no J(Ref.: . . . .)
  - **(X)** full rot-vib treatment (number of ν/J levels: ground state ν=0-14, Lyman band 24 level + Werner band 10 level . . . . Ref.: . . . .)
- **(X)** H_2 dissociation (Ref.: . . . .)
- **(X)** H_2 formation (Ref.:rbitrary distribution . . . .)
- **(X)** CR heating ($\Lambda_{cr} = 61610 \times \zeta$ (cm^{-1}H-particle^{-1} s^{-1}) with CR destruction rate $\zeta = 5 \times 10^{-17}$ . . . .)
- **(X)** PE heating (Ref.: Bakes & Tielens, 1994, ApJ, 427, 822 . . . .)
- **( )** XR heating (Ref.: . . . .)
- **( )** PAH heating (Ref.: . . . .)
- **( )** . . . .
- **( )** . . . .

12.6 Radiative Transfer

12.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(X) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

( ) via simple exponentials (Ref.: ....)

(X) via biexponentials (e.g. Sternberg & Dalgarno 1995) (Ref.: ....)

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

Dust Properties

(X) treatment of radiative transfer (Ref.: Hollenbach, Takahashi & Tielens, ApJ, 377, 192 (1991))

(X) grain size distribution (PAHs as chemical species: MRN size distribution for $30 \leq N_C \leq 1500$. For photoelectric heating: see Bakes & Tielens, 1994, ApJ, 427, 822)

(X) extinction/scattering law in UV(MRN + Draine-Lee model assumed in calculating the dust attenuation functions ....)

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

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

Shielding of H_2

( ) No

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

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

(X) detailed solution (Ref.: Störzer et al. 1996 ....)

Shielding of CO

( ) No

(X) shielding factors (Ref.: van Dishoeck & Black, ApJ 334, 771 (1988) ....)

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

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

( ) Isotope selective photodissociation(Ref.: van Dishoeck & Black, ApJ 334, 771 (1988) ....)

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

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

(X) Voigt (approximately, Federman,Glassgold, Kwan 79, pure Gaussion core plus Lorentzian wings)

( ) Box (width: ....)

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

12.6.2 Radiative Transfer in Cooling Lines

Method:

(X) Escape probability (Ref.: Sternberg & Dalgarno, ApJ, 338, 197-233, 1989
$\beta(\vec{r}) =$ . . . .)
( ) other . . . .

( ) Solution of RT equation in given geometry

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

Remarks . . . .)

Cooling Lines included:

(X) O (63μ,146μ,44μ . . . .)
( ) ^{12}CO rotational lines (up to J:);
(X) $^{12}C^+$ (158 μ)
(X) ^{12}C (610 μ,370 μ,230μ . . . .)
(X) Si^+ (35 μ)
( ) ^{13}CO rotational lines (up to J:)
( ) OH rotational lines (. . . .)
( ) H_2O rotational lines (. . . .)
( ) . . . .
( ) . . . .

12.6.3 Radiative Transfer of Observable Line Intensities

Method:

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

(X) Solution of RT equation in given geometry

Remarks . . . .)

Lines included:

(X) O (no. of lines: 3)
(X) C (no. of lines: 3)

(X) C^+ (no. of lines: 1)
( ) CO (no. of lines:)
( ) ^{13}CO (no. of lines:)
( ) $C^{18}O$ (no. of lines:)
( ) $^{13}C^{18}O$ (no. of lines: 50)
( ) H_2O (no. of lines:...........)
( ) $H_2{}^{18}O$ (no. of lines:...........)
( ) other: HCO^+ (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 (. . . .)
( ) Box (width: . . . .)
( ) other (Ref.: . . . .)

( ) antenna characteristics included

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

( ) ....

( ) turbulence included: Gaussian line width > thermal line width ....

( ) ....

( ) ....

12.7 Rate Coefficients

Collision Rates

- **(X)** H-H (Ref.: ....)
- **(X)** H-H_2(Ref.:Mandy & Martin, APJS, 86, 199, 1993, Lepp et al , unpublished)
- **(X)** H_2-H^+ (Ref.:Gerlich, 1990, J Chem Phys, 92, 2377 ....)
- **(X)** H_2-*e* (Ref.: ....)
- **(X)** H_2-H_2 (Ref.: ....)
- **( )** CO-H (Ref.: ....)
- **( )** CO-H_2 (Ref.:Schinke et al, 1985, ApJ 299,939 ....)
- **( )** CO-*e* (Ref.:Elitzur, 1977, A&A 57, 179 ....)
- **( )** C^+-*e* (Ref.: ....)
- **( )** C^+-H_2 (Ref.:Flower and Launay, 1977, J.Phys. B, 10/5, 879 ....)
- **( )** C^+-H (Ref.:Flower and Launay, 1977, J.Phys. B, 10/5, 879 ....)
- **( )** OI-*e* (Ref.: ....)
- **(X)** OI-H_2 (Ref.:Launay and Roueff, 1977, J.Phys. B, 10, 879, Jaquet et al, 1992, J.Phys.B, 25, 285 ....)
- **(X)** OI-H (Ref.:Launay and Roueff, 1977, J.Phys. B, 10, 879, Jaquet et al, 1992, J.Phys.B, 25, 285 ....)
- **(X)** C-H (Ref.:Launay and Roueff, 1977, A&A, 56, 289 ....)
- **( )** ...-H (Ref.: ....)
- **( )** C-H_2 (Ref.: ....)
- **( )** OH-H_2 (Ref.: ....)
- **( )** He-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.: . . . .
. . . .)

(X) H_2 (Ref.: . . . .
. . . .)

(X) C (Ref.: . . . .
. . . .)

(X) O (Ref.: . . . .
. . . .)

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

(X) C^+ (Ref.: . . . .
. . . .)

( ) H_2O (Ref.: . . . .
. . . .)

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

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

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

12.8 Output

PDR code:

(X) abundance profiles over (A_V/depth) . . . .

(X) column density over (A_V/depth) . . . .

(X) temperature profile over (A_V/depth) . . . .

(X) heating and cooling over (A_V/depth) and the contribution by different processes discussed above . . . .

(X) chemical rates over (A_V/depth) . . . .

12.9 Numerics

Gridded variables

- **( )** frequency/wavelength
- **( )** temperature
- **(X)** spatial coordinate(s) (H_2 column density is the independent variable
- **( )** velocity
- **( )** time
- **( )** . . . .
- **( )** . . . .

. . . .

. . . .

Numerical method to solve the chemical network: rate equations solved using Newton-Raphson method

(Sternberg & Dalgarno, 1995).

. . . .

. . . .

. . . .

(Ref.: Routine DGESV from LAPACK, Numerical Recipes, Press et al. . . . .)

Numerical method to solve the thermal balance: root finding method of Anderson, Bjoerck and King

. . . .

. . . .

. . . .

(Ref.:)

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

In PDR model (in order to calculate the cooling by line emission): escape probability method . . . .

. . . .

(Ref.: Sternberg & Dalgarno (1989) . . . .)

Description of the iteration schemes . . . .

. . . .

. . . .

. . . .

. . . .

Numerical parameters to tune convergence/computation speed/accuracy

- **(X)** step size (Burlisch-Stoer algorithm (Press et al., Num. Recipes) . . . .)
- **(X)** accuracy goal (. . . .)
- **(X)** starting solution (start temperature . . . .)
- **( )** methods for convergence acceleration (. . . .)
- **( )** parallelized code(. . . .)
- **( )** . . . .
- **( )** . . . .

Usage of numerical standard routines/packages: code is self-contained; uses subroutines from the Numerical Recipes in F

- **( )** NAG
- **(X)** BLAS
- **(X)** SLATEC
- **( )** ODEPACK (LSODE)
- **( )** LINPACK
- **(X)** Numerical Recipes in Fortran . . . .
- **( )** . . . .

12.10 Misc

Hardware

- **(X)** x86 PC . . . .
- **( )** SUN . . . .
- **( )** HP . . . .
- **( )** DEC . . . .
- **( )** IBM . . . .
- **( )** . . . .

Operating System

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

Compiler

- **Fortran**
  - **(X)** g77
  - **( )** g90
  - **( )** Absoft f77
  - **( )** Absoft f90
  - **( )** Sun Workshop f77
  - **( )** Sun Workshop f90
  - **( )** . . . .
  - **( )** . . . .
- **C/C++**
  - **( )** gcc
  - **( )** Sun Workshop C/C++ compiler
  - **( )** . . . .
  - **( )** . . . .
- **( )** other (. . . .)

Memory Requirements (MB): $\approx$ 1000 . . . .

Processor Speed (MHz): 3.2 GHz . . . .

Standard computation time for one model: 1 minute . . . .

12.11 Remarks

. . . .

. . . .

. . . .

. . . .

. . . .

. . . .

. . . .

. . . .

Chapter 13

UCL_PDR

13.1 Model Identification

Name of the Model . . . . UCL_PDR Model

List of Authors . . . . Serena Viti, Wing-Fai Thi, Tom Bell

Institute . . . . University College London

Contact Email . . . . tab@star.ucl.ac.uk

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

Papadopoulos, Thi & Viti 2002, ApJ, 579, 270 . . . .

Taylor, Hartquist & Williams 1993, MNRAS, 264, 929 . . . .

Additional Info . . . .

. . . .

. . . .

. . . .

13.2 Geometry

( ) spherical

(X) plane-parallel (semi-infinite)

( ) plane-parallel (finite)

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

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

Density

- **(X)** homogeneous
- **(-)** density gradient (Eq.: . . . . Please see remarks)
- **( )** velocity field (Eq.: . . . .)
- **( )** time dependent geometry (. . . .)

13.3 Radiation Field

( ) isotropic[1] (Ref.: . . . .)

(X) uni-directional (Ref.: . . . . Taylor et al. 1993)

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

13.3.1 Radiation sources

(X) external source

- **(X)** Habing field
- **( )** Draine field
- **( )** Other (Ref.: . . . .)
- **( )** Detailed spectral energy distribution (Ref.: . . . .)

(-) internal source

- **( )** Habing field
- **( )** Draine field
- **(-)** Other (Ref.: . . . . Please see remarks)
- **( )** detailed spectral energy distribution (Ref.: . . . .)

13.4 Chemistry

(X) time dependent solution (Ref.: . . . . Papadopoulos et al. 2002)

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

Underlying Database

- **(X)** UMIST95
- **( )** UMIST99

[1]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 just drops exponentially with τ. In an isotropic radiation field one has to integrate over all angles to obtain $\bar{I}_\nu$.

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

Extension of database:

Several reaction rates have been adjusted over the years . . . .
Ref.: Papadopoulos et al. 2002 . . . .
Ref.: . . . .

(X) fixed number of included species (number: 128)

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

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

(X) depletion on grains/ice included (Ref.: . . . . Coded but not used)

(X) formation of H_2 on grains (Ref./Eq.: . . . . de Jong 1977, A&A, 55, 137)

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

( ) desorption mechanisms included

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

(X) metallicity effects included

(X) scaling law[2] for elemental abundances (Eq./Ref.: . . . . $X(i)=Z\times X(i)$)
(X) scaling law[3] for dust abundance (Eq./Ref.: . . . . $n_g \propto Z$)
(X) scaling law[3] for PAH abundance (Eq./Ref.: . . . . PAHs depletion $\propto Z$)
(X) metallicity dependent heating rates (Ref.: . . . Wolfire et al. 1995, ApJ, 453, 673)
(X) metallicity dependent cooling rates (Ref.: . . . . . Computed self-consistently)

( ) isotopomers included

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

( ) other . . . .

( ) other . . . .

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

13.5 Thermal Balance

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

(X) temperature determined from energy balance

Cooling Functions

- **(X)** gas-grain cooling (Ref.: . . . . Kamp & van Zadelhoff 2001, A&A, 373, 641)
- **(X)** radiative line cooling (details in section 13.6.2)
- **( )** . . . .
- **( )** . . . .

Heating Functions

- **(X)** H_2^* vibrational deexcitation
  - **(X)** single line approx. (Ref.: Hollenbach & McKee 1979, ApJS, 41, 555)
  - **( )** only ν-levels but no J (Ref.: . . . .)
  - **( )** full rot-vib treatment (number of ν/J levels: . . . . Ref.: . . . .)
- **(X)** H_2 dissociation (Ref.: . . . . Tielens & Hollenbach 1985, ApJ, 291, 772)
- **(X)** H_2 formation (Ref.: . . . . Tielens & Hollenbach 1985)
- **(X)** CR heating (Ref.: . . . . Clavel, Viala & Bel 1978, A&A, 65, 435)
- **(X)** PE heating (Ref.: . . . . Tielens & Hollenbach 1985)
- **(X)** XR heating (Ref.: . . . . Wolfire et al. 1995, ApJ, 453, 673)
- **(X)** PAH heating (Ref.: . . . . Wolfire et al. 1995)
- **(X)** Carbon ionisation heating (Ref.: . . . . Tielens & Hollenbach 1985)
- **(X)** Turbulence heating (Ref.: . . . . Black 1997, Interstellar Processes, 731)

13.6 Radiative Transfer

13.6.1 UV transfer

( ) RT solved for precomputed density and temperature structure

(X) RT solved selfconsistently with chemical and thermal balance equations

Attenuation of the photodissociation rates

- **(X)** via simple exponentials (e.g. like in UMIST) (Ref.: . . . . Taylor et al. 1993 . . . .)
- **( )** via biexponentials (e.g. Sternberg & Dalgarno 1995) (Ref.: . . . .

. . . .)

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

Dust Properties

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

(X) grain size distribution (Ref.: . . . . Mean average used)

(X) extinction/scattering law in UV (Ref.: . . Savage et al. 1977, ApJ, 216, 291)

(X) albedo (Ref.: . . . . Observational value used)

(X) scattering function (. . Wagenblast & Hartquist 1989, MNRAS, 237, 1019)

Shielding of H_2

( ) No

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

(X) single line (Ref.: . . . . . Federman, Glassgold & Kwan 1979, ApJ, 227, 466)

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

Shielding of CO

( ) No

(X) shielding factors (Ref.: . . . . van Dishoeck & Black 1988, ApJ, 334, 771)

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

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

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

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

(X) Gaussian (doppler parameter: $\Delta v_d = \sqrt{v_{turb}^2 + 6^{-4}T}$ . . . .)

( ) Voigt

( ) Box (width: . . . .)

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

13.6.2 Radiative Transfer in Cooling Lines

Method:

(X) Escape probability (Ref.: de Jong, Boland & Dalgarno 1980, A&A, 91, 68)

$\beta(\vec{r}) = (1 - \exp(-2.34\tau))/(4.68\tau)$ for $\tau < 7$ . . . .

$\beta(\vec{r}) = (4\tau[\ln(\tau/\sqrt{\pi})]^{1/2})^{-1}$ for $\tau \geq 7$ . . . .

( ) Solution of RT equation in given geometry

(X) IR pumping (e.g. OI) (Ref.: . . . . Goldsmith & Carroll 1981, ApJ, 245, 891)

Remarks . . . .)

Cooling Lines included:

- **(X)** O (63μ, 146μ, 44μ, ...)
- **(X)** ^{12}CO rotational lines (up to J: 11→10)
- **(X)** $^{12}C^+$ (158μ)
- **(X)** ^{12}C (610μ, 370μ, 230μ, ...)
- **( )** Si^+ (35μ)
- **( )** OH rotational lines (up to J:........)
- **( )** H_2O rotational lines (up to J:........)
- **(X)** H_2 rotational lines (Ref.: . Martin, Schwarz & Mandy 1996, ApJ, 461, 265)
- **(X)** O 6300Å metastable line (Ref.:Sternberg & Dalgarno 1989, ApJ, 338, 197)
- **(X)** Lyα metastable line (Ref.: . . . . Tielens & Hollenbach 1985)

13.6.3 Radiative Transfer of Observable Line Intensities

Method:

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

( ) Solution of RT equation in given geometry

Remarks RT only considered for cooling lines . . . .

Lines included:

- **(X)** O (no. of lines: 3)
- **(X)** C (no. of lines: 3)
- **(X)** C^+ (no. of lines: 2)
- **(X)** CO (no. of lines: 12)
- **( )** ^{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: . . . .

. . . .)

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

. . . .)

(X) 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.: . . . .)

( ) . . . .

( ) . . . .

13.7 Rate Coefficients

Collision Rates

- **( )** H-H (Ref.: . . . .)
- **(X)** H_2-H (Ref.: . . . . Martin, Schwarz & Mandy 1996, ApJ, 461, 265)
- **( )** H_2-H^+ (Ref.: . . . .)
- **( )** H_2-e (Ref.: . . . .)
- **( )** H_2-H_2 (Ref.: . . . .)
- **(X)** CO-H (Ref.: . . . . Balakrishnan, Yan & Dalgarno 2002, ApJ, 568, 443)
- **(X)** CO-H_2 (Ref.: . . . . Flower 2001, J.Phys.B., 34, 2731)
- **(X)** CO-e (Ref.: . . . . Saha et al. 1981, Phys.Rev.A., 23, 2926)
- **(X)** C-H (Ref.:Flower 1990, Molecular Collisions in ISM, Cambridge U. Press)
- **(X)** C-H_2 (Ref.: . . . . Schröder et al. 1991)
- **(X)** C-e (Ref.: . . . . Johnson et al. 1987, J.Phys.B., 20, 2553)
- **(X)** C^+-H (Ref.: . . . . Launay & Roueff 1977, J.Phys.B., 10, 879)
- **(X)** C^+-H_2 (Ref.: . . . . Tielens & Hollenbach 1985)
- **(X)** C^+-e (Ref.: . . . . Blum & Pradhan 1992, ApJS, 80, 425)
- **(X)** OI-H (Ref.: . . . . Launay & Roueff 1977)
- **(X)** OI-H_2 (Ref.: . . . . Jaquet et al. 1992, J.Phys.B., 25, 285)
- **(X)** OI-H^+ (Ref.: . . . . Pequignot 1990, A&A, 231, 499)
- **(X)** OI-e (Ref.: . . . . Liseau et al. 1999, A&A, 344, 342)
- **( )** ...-H (Ref.: . . . .)
- **( )** ...-H (Ref.: . . . .)
- **( )** ...-H_2 (Ref.: . . . .)
- **( )** ...-H_2 (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.: . . . .)

(X) CO-He (Ref.: . . . . McKee et al. 1982, ApJ, 259, 647)
(X) C-He (Ref.: . . . . Staemmler & Flower 1991, J.Phys.B., 24, 2343)
(X) O-He (Ref.: . . . . Monteiro & Flower 1987, MNRAS, 228, 101)
( ) ...... (Ref.: . . . .)

A-values

(X) CO (Ref.: . . . . Varberg & Evenson 1992, ApJ, 385, 763
. . . .)
(X) H_2 (Ref.: . . . . Martin, Schwarz & Mandy 1996, ApJ, 461, 265
. . . .)
(X) C (Ref.: . . . . Tielens & Hollenbach 1985
. . . .)
(X) O (Ref.: . . . . Galavis, Mendoza & Zeippen 1997, A&A, 123, 159
See also: . . . . Silva & Viegas 2002, MNRAS, 329, 135)
( ) OH (Ref.: . . . .
. . . .)
(X) C^+ (Ref.: . . . . Nussbaumer & Storey 1983, A&A, 126, 785
. . . .)
( ) H_2O (Ref.: . . . .
. . . .)
( ) ......(Ref.: . . . .
. . . .)
( ) ...... (Ref.: . . . .
. . . .)
( ) ...... (Ref.: . . . .
. . . .)

13.8 Output

(X) abundance profiles over (A_V/depth)

(X) temperature profile over (A_V/depth)

(X) emitted intensities (details at 13.6.3)

( ) opacities at linecenters (. . . .)

( ) . . . .

( ) . . . .

( ) . . . .

13.9 Numerics

Gridded variables

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

Gridding strategies: . . . .

The spatial coordinate (cloud depth) grid is adapted such that the variation in the . . . .

H_2 self-shielding function is small (i.e. $<$10%) . . . .

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

Stiff integration using the GEAR package . . . .

. . . .

(Ref.: Hindmarsh, A.C., UCID-30001, Rev. 3, Lawrence Livermore Laboratory . . . .)

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

Modified version of Ridder's method . . . .

. . . .

(Ref.: Press et al. 1992, Numerical Recipes in Fortran, Cambridge University Press)

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

. . . .

. . . .

(Ref.: . . . .)

Description of the iteration schemes . . . .

. . . .

. . . .

. . . .

. . . .

Numerical parameters to tune convergence/computation speed/accuracy

(X) step size (Maximum depth step in adaptive spatial grid is A_V=0.1 mags . .)

(X) accuracy goal (Temperature accurate to 2.5K in thermal balance iteration .)

( ) starting solution (. . . .)

(X) methods for convergence acceleration

(Maximum and minimum temperatures in thermal balance iteration . . . .)

( ) parallelized code (. . . .)

( ) . . . .

Usage of numerical standard routines/packages

( ) NAG

( ) BLAS

( ) SLATEC

( ) ODEPACK (LSODE)

( ) LINPACK

(X) GEAR

( ) . . . .

13.10 Misc

Hardware

( ) x86 PC . . . .

( ) SUN . . . .

( ) HP . . . .

( ) DEC . . . .

( ) IBM . . . .

(X) Optimised for ALPHA & x86 PC . . . .

Operating System

(X) Linux . . . .

( ) Solaris . . . .

( ) HP-UX . . . .

( ) MacOS . . . .

( ) other UNIX . . . .

( ) MS Windows . . . .

(X) ALPHA . . . .

Compiler

Fortran

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

C/C++

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

( ) other (. . . .)

Memory Requirements (MB): 128MB . . . .

Processor Speed (MHz): 900MHz . . . .

Standard computation time for one model: Under 10 minutes to reach A_V=20 on a 900MHz AMD Athlon machine with 128Mb of memory . . . .

13.11 Remarks

Since the model uses a semi-infinite slab geometry, internal radiation sources are . . . identical to external radiation sources, so both can be modelled . . . .

. . . .

Although a homogeneous cloud density is currently used in the model, the option of using a depth-dependent density profile is coded for as well . . . .

. . . .

. . . .

. . . .