Betreff: PDR workshop - request for benchmark calculations

Dear Participant-

We would like to start collecting output results from the various PDR codes around the world in preparation for the workshop. We would like to start by requesting output that we specify below, for a single model with the following assumed input parameters. These should be computations assuming a semi-infinite plane-parallel model. (Please note that the total number of benchmark computations we are asking for is 8 different models. We chose a two-step approach: one first priority model is calculated at first with the input parameters given below, and the results beeing sent to M.Röllig (roellig@ph1.uni-koeln.de) until the end of this week (deadline: Friday, 12.March 2004). The deadline for the 7 remaining models is Thursday, 25. March 2004.(the input parameter for this 7 models are given at the end of this email.)

Input parameters:

total hydrogen density n = n(H)+2n(H2) = 1e3 cm^-3
assumed constant throughout.

gas temperature Tgas = 50 K
assumed constant throughout.

dust temperature Tdust= 20 K
assumed constant throughout.

Radiation field 10 times the Draine (1978) field.
Please take care to note that for a semi-infinite plane parallel cloud the CO dissociation rate at the cloud surface should equal 1e-9 s^-1, if for fully optically thin conditions (for which a point is exposed to the full 4pi steradians as opposed to just 2pi at the cloud surface) the CO dissociation rate is 2e-10 s^-1 for a unit Draine field.

cosmic-ray ionization rate zeta = 5e-17 s^-1

absorption line b-value = 1 km s^-1 (emission/cooling lines also)

Please assume that the
visual extinction A_V = 6.289e-22*N_Htotal

For the chemistry computation please restrict to the
following limited set of He, C, and O species:
h h+ h2 h2+ h3+
o o+ oh+ oh o2 o2+ h2o h2o+ h3o+
c c+ ch ch+ ch2 ch2+ ch3 ch3+ ch4 ch4+ ch5+ co co+ hco+
he he+

with abundances at

He = 0.1
C = 1.00e-4
O = 3.00e-4

(Please set all other elements to zero, and also
exclude PAHs).

Please use chemical rate coefficients, and photorates
as given in the attached file "rate99_edited_incl_crp.dat"
This file is the UMIST99 data base as edited by
A. Sternberg to include several updates and corrections.
For the comparison tests we are attempting it is
important that everyone use the same rate coefficients
as specified in this data file.

For the special case of H2, if your code does not
explicitly calculate the unattenuated photodissociation
rates (by summing over oscillator strengths etc) please
assume that the unattenuated H2 photodissociation rate
in a unit Draine field is equal to 5.18e-11 s^-1,
so that at the surface of a semi-infinite cloud
for 10xDraine the H2 dissociation rate is 2.59e-10 s^-1.

For the dust attenuation factor in the H2 dissociation
rate please assume exp(-k*A_V) with k=3.02.

Please assume an H2 formation rate coefficient

R = 3e-18*T^1/2 = 2.121e-17 cm^3 s^-1

Please include the cosmic-ray induced photodestruction
rates as given in the attached rate99_edited_incl_crp.dat file.

We would like to focus on several specific output quantities.
For the comparison it would be useful if you could send us the
following information divided into separate ascii files as follows,

Output files requested:

1) local absolute volume densities (cm^-3) versus cloud depth,
format(12(1pe10.3))

z(cm) A_V H H2 C+ C CO O O2 CH OH e

2) integrated columns as functions of depth from cloud surface,

z(cm) A_V H H2 C+ C CO O O2 CH OH e

3) Local H2 and CO dissociation rates, and C ionization rate (s^-1)
format(5(1pe10.3))

z(cm) A_V H2dis COdis Cion

4) local emissivities (erg s^-1 cm^-3) in cooling transitions
and local photoelectric heating rate (erg s^-1 cm^-3)
assuming a fixed gas temperature of 50K and dust temp of 20K.
format(8(1pe10.3)

z(cm) A_V CII158 OI63 OI146 CI610 CI370 photoelectric

5) Finally, please also send the values of the total resulting surface
brightnesses (erg s^-1 cm^-2 sr^-1) for the above five cooling lines.

The input parameters for the 7 remaining models are:

MODEL 2
total density n=10^3 cm^-3

UV field \chi=10^5 [units of the standard Draine field]
temperature fixed T= 50 K, Tdust=20K

MODEL 3
total density n=10^5.5 cm^-3
UV field \chi=10 [units of the standard Draine field]
temperature fixed T= 50 K, Tdust=20K

MODEL 4
total density n=10^5.5 cm^-3
UV field \chi=10^5 [units of the standard Draine field]
temperature fixed T= 50 K, Tdust=20K

All groups who are able to compute the energy balance should calculate the following 4 models. Additionally to the output files requested above an extra file for the temperatures (gas and dust) should be added:
format(4(1pe10.3)

z(cm) A_V T_gas T_dust

MODEL 5
total density n=10^3 cm^-3
UV field \chi=10 [units of the standard Draine field]
temperature calculated

MODEL 6
total density n=10^3 cm^-3
UV field \chi=10^5 [units of the standard Draine field]
temperature calculated

MODEL 7
total density n=10^5.5 cm^-3
UV field \chi=10 [units of the standard Draine field]
temperature calculated

MODEL 8
total density n=10^5.5 cm^-3
UV field \chi=10^5 [units of the standard Draine field]
temperature calculated

All the other parameters are the same as given above for the first priority model.

Summary:

Deadline for the fist model: 12.March 2004
Deadline for the reamining models: 25. March 2004

If there are any open questions regarding this configurations please
contact me - I will answer as quickly as possible.

Markus Röllig

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