

# Chemical modeling: *Quick guide to running TRICKS*



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# Chemical model

- **TRICKS** = *Trainer for Interstellar Chemical Kinetics Simulations*
- Has a full gas-phase chemistry and a primitive surface chemistry
- It is based on my full-function astrochemical code:  
**MAGICKAL** = *Model for Astrophysical Gas and Ice Chemical Kinetics and Layering*
- Written in Fortran (77)
- Can be compiled using Intel Fortran (best) or f77, g77, gfortran compilers (ok)
- Run on Linux systems
- Available at my website: <https://garrodgroup.as.virginia.edu/resources>

**tricks\_v2.3.zip** ← Contains all files needed to run the code

**tricks\_v2.3\_outputs.zip** ← The output files, if you just want to look at those

# Platform

- TRICKS is written in Fortran (77-style), and is supposed to run on a Linux platform.
- You may already have something like the Intel Fortran, gfortran, f77, or g77 Fortran compiler available at your own institution. Use one of those if possible.
- If you want to run TRICKS on your own machine, you will need a version of Fortran. You may find a workable solution at the following website (not mine, I take no responsibility for content):

<https://gcc.gnu.org/wiki/GFortranBinaries#MacOS>

- TRICKS is set up to use “gfortran”, if you have a different compiler installed, you will have to make a minor edit to the “makefile”, which contains a set of commands used to compile the code.

# Linux cheat sheet


- `cd` = change directory (folder)
  - E.g. `cd ../../programs`
- `ls` = list contents of directory
- `pwd` = print working directory = “where am I?”
- `mkdir` = make directory
  - E.g. `mkdir new_folder`
- `cp` = copy something to something else or somewhere else
  - E.g. `cp file1 file2` (makes a differently named copy in the same folder)
  - E.g. `cp file1 ../../programs` (makes an identical copy in another folder)
  - E.g. `cp file1 ../../programs/file2` (makes different copy in another folder)
- `mv` = move something to something/somewhere else  
(same as copy, but it deletes the original)
- `rm` = remove (delete) – BE VERY CAREFUL! There is NO “undelete” operation.
- `exit` = disconnect from remote machine

# If you have a different compiler installed...

In the "Makefile", change the compiler that will be used, by adding/removing a "#" (comment character):

```
OBJECTS = dgear.o trx_shield.o trx_io.o tricks.o
FC = ifort
#FC = ifort -f77rtl
#FC = gfortran
#FC = f77
#FC = g77

tricks: $(OBJECTS)
        $(FC) $(OBJECTS) -o do_tricks
~
~
~
```



You can use vi or vim to edit, i.e. type the following in a terminal:

```
vi Makefile
```

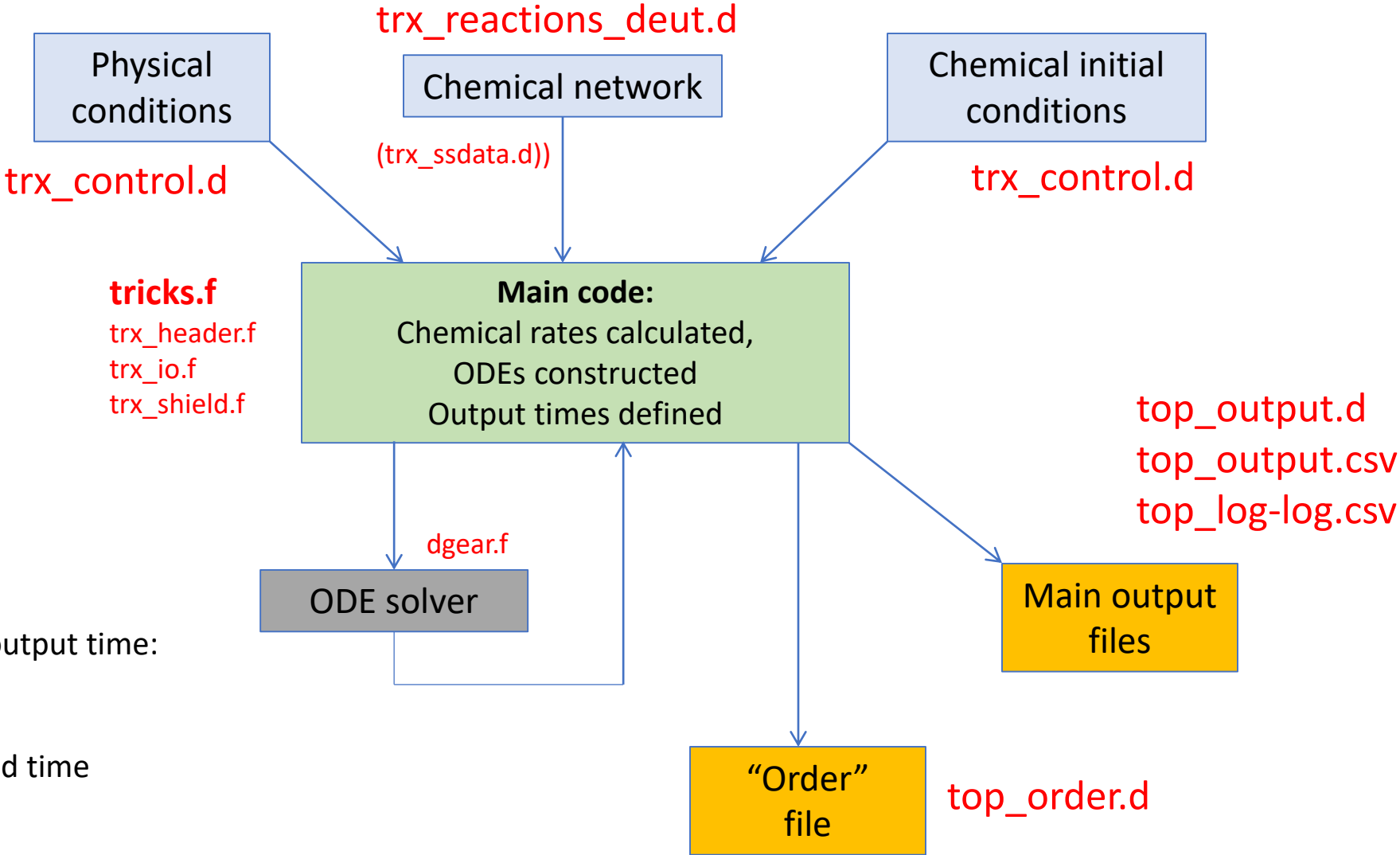
Comment/uncomment compiler instruction:

[arrow keys]	-	move cursor
i	-	enter edit mode
#	-	write "#"
[arrow keys]	-	move cursor
[backspace]	-	delete other"#"
[esc]	-	exit edit mode

Command within vi to save (write) and exit (quit):

```
:
wq
```

# Components of a (gas-phase) chemical model



One solver call for each output time:

Solver takes multiple *timesteps* to reach desired time

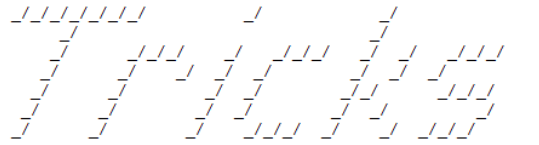
# Running “tricks”

Start in a Linux terminal.

Put the zipped file into a directory/folder where you want to run the code, then follow the instructions on the right...

(The instructions are for the v2.1 version of the code, but are fine for the latest version)

```
-bash-4.2$ls ← List what's in the current directory
tricks_v2.1.zip
-bash-4.2$
-bash-4.2$mkdir tricks ← Make a directory to run the code in
-bash-4.2$
-bash-4.2$cp tricks_v2.1.zip tricks ← Copy zip file to the new directory
-bash-4.2$
-bash-4.2$cd tricks ← Enter that directory
-bash-4.2$
-bash-4.2$unzip tricks_v2.1.zip ← Unzip the program files into current dir.
Archive:  tricks_v2.1.zip
  inflating: dgear.f
  inflating: do_tricks
  inflating: Makefile
  inflating: tricks.f
  inflating: trx_control.d
  inflating: trx_header.f
  inflating: trx_io.f
  inflating: trx_reactions_deut.d
  inflating: trx_shield.f
  inflating: trx_ssdata.d
-bash-4.2$
-bash-4.2$make ← Compile the code, based on instructions in the “Makefile”
ifort -c -o dgear.o dgear.f
ifort -c -o trx_shield.o trx_shield.f
ifort -c -o trx_io.o trx_io.f
ifort -c -o tricks.o tricks.f
ifort dgear.o trx_shield.o trx_io.o tricks.o -o do_tricks
-bash-4.2$
-bash-4.2$./do_tricks ← Run the executable
```



-----  
\*Trainer for Interstellar Chemical Kinetics Simulations\*  
v2.1 (2022)  
-----

trx\_reactions\_deut.d  
-----

```
IT= 2, TIME= 1.000000E+00 yrs
IT= 3, TIME= 1.333521E+00 yrs
IT= 4, TIME= 1.778279E+00 yrs
IT= 5, TIME= 2.371374E+00 yrs
IT= 6, TIME= 3.162278E+00 yrs
IT= 7, TIME= 4.216965E+00 yrs
IT= 8, TIME= 5.623413E+00 yrs
IT= 9, TIME= 7.498942E+00 yrs
IT= 10, TIME= 1.000000E+01 yrs
IT= 11, TIME= 1.333521E+01 yrs
IT= 12, TIME= 1.778279E+01 yrs
IT= 13, TIME= 2.371374E+01 yrs
IT= 14, TIME= 3.162278E+01 yrs
IT= 15, TIME= 4.216965E+01 yrs
IT= 16, TIME= 5.623413E+01 yrs
IT= 17, TIME= 7.498942E+01 yrs
IT= 18, TIME= 1.000000E+02 yrs
IT= 19, TIME= 1.333521E+02 yrs
IT= 20, TIME= 1.778279E+02 yrs
IT= 21, TIME= 2.371374E+02 yrs
IT= 22, TIME= 3.162278E+02 yrs
IT= 23, TIME= 4.216965E+02 yrs
IT= 24, TIME= 5.623413E+02 yrs
IT= 25, TIME= 7.498942E+02 yrs
IT= 26, TIME= 1.000000E+03 yrs
IT= 27, TIME= 1.333521E+03 yrs
IT= 28, TIME= 1.778279E+03 yrs
IT= 29, TIME= 2.371374E+03 yrs
IT= 30, TIME= 3.162278E+03 yrs
IT= 31, TIME= 4.216965E+03 yrs
IT= 32, TIME= 5.623413E+03 yrs
IT= 33, TIME= 7.498942E+03 yrs
IT= 34, TIME= 1.000000E+04 yrs
IT= 35, TIME= 1.333521E+04 yrs
IT= 36, TIME= 1.778279E+04 yrs
IT= 37, TIME= 2.371374E+04 yrs
IT= 38, TIME= 3.162278E+04 yrs
IT= 39, TIME= 4.216965E+04 yrs
IT= 40, TIME= 5.623413E+04 yrs
IT= 41, TIME= 7.498942E+04 yrs
IT= 42, TIME= 1.000000E+05 yrs
IT= 43, TIME= 1.333521E+05 yrs
IT= 44, TIME= 1.778279E+05 yrs
IT= 45, TIME= 2.371374E+05 yrs
IT= 46, TIME= 3.162278E+05 yrs
IT= 47, TIME= 4.216965E+05 yrs
IT= 48, TIME= 5.623413E+05 yrs
IT= 49, TIME= 7.498942E+05 yrs
IT= 50, TIME= 1.000000E+06 yrs
IT= 51, TIME= 1.333521E+06 yrs
IT= 52, TIME= 1.778279E+06 yrs
IT= 53, TIME= 2.371374E+06 yrs
IT= 54, TIME= 3.162278E+06 yrs
IT= 55, TIME= 4.216965E+06 yrs
IT= 56, TIME= 5.623413E+06 yrs
IT= 57, TIME= 7.498942E+06 yrs
IT= 58, TIME= 1.000000E+07 yrs
```

DONE

# Running “tricks”

This is what you should see on your screen (terminal) as the code runs.

It should take about a minute or less to run.



# Chemical networks (OSU, TRICKS, etc.)

	q	H	He	C	N	O	Si	S	Fe	Na	Mg	Cl	P	D		
C	0	0	0	1	0	0	0	0	0	0	0	0	0	0	*	1*
C10	0	0	0	10	0	0	0	0	0	0	0	0	0	0	*	2*
C2	0	0	0	2	0	0	0	0	0	0	0	0	0	0	*	3*
C2D	0	0	0	2	0	0	0	0	0	0	0	0	0	1	*	4*
C2H	0	1	0	2	0	0	0	0	0	0	0	0	0	0	*	5*
C2H2	0	2	0	2	0	0	0	0	0	0	0	0	0	0	*	6*
C2H2D	0	2	0	2	0	0	0	0	0	0	0	0	0	1	*	7*
C2H3	0	3	0	2	0	0	0	0	0	0	0	0	0	0	*	8*
C2H3CN	0	3	0	3	1	0	0	0	0	0	0	0	0	0	*	9*
C2H3D	0	3	0	2	0	0	0	0	0	0	0	0	0	1	*	10*
C2H3OH	0	4	0	2	0	1	0	0	0	0	0	0	0	0	*	11*
C2H4	0	4	0	2	0	0	0	0	0	0	0	0	0	0	*	12*
C2H4OH	0	5	0	2	0	1	0	0	0	0	0	0	0	0	*	13*
C2H5	0	5	0	2	0	0	0	0	0	0	0	0	0	0	*	14*
C2H5D	0	5	0	2	0	0	0	0	0	0	0	0	0	1	*	15*
C2H5O	0	5	0	2	0	1	0	0	0	0	0	0	0	0	*	16*
C2H5OH	0	6	0	2	0	1	0	0	0	0	0	0	0	0	*	17*
C2H6	0	6	0	2	0	0	0	0	0	0	0	0	0	0	*	18*
C2HD	0	1	0	2	0	0	0	0	0	0	0	0	0	1	*	19*
C2N	0	0	0	2	1	0	0	0	0	0	0	0	0	0	*	20*
C2O	0	0	0	2	0	1	0	0	0	0	0	0	0	0	*	21*
C2S	0	0	0	2	0	0	0	1	0	0	0	0	0	0	*	22*
C3	0	0	0	3	0	0	0	0	0	0	0	0	0	0	*	23*
C3D	0	0	0	3	0	0	0	0	0	0	0	0	0	1	*	24*
C3H	0	1	0	3	0	0	0	0	0	0	0	0	0	0	*	25*
C3H2	0	2	0	3	0	0	0	0	0	0	0	0	0	0	*	26*
C3H2D	0	2	0	3	0	0	0	0	0	0	0	0	0	1	*	27*
C3H3	0	3	0	3	0	0	0	0	0	0	0	0	0	0	*	28*

## REACTION FILE:

Chemical species in the network are listed at the top of the reaction file.

Chemical species usually ordered alphabetically.

Charge and mass defined for each species.

# Chemical networks (OSU, TRICKS, etc.)

CD+	C	D+
CH+	C	H+
C	C+	e-
C2H2	C2H2+	e-
C2H2D	C2H2D+	e-
C2H3D	C2H3D+	e-
C2H4	C2H4+	e-
C2H5D	C2H5D+	e-
C2H5OH	C2H5OH+	e-
C2HD	C2HD+	e-
C3H3D	C3H3D+	e-
C3H4	C3H4+	e-
C4H2	C4H2+	e-
C4HD	C4HD+	e-
CD3	CD3+	e-
CD3OD	CD3OD+	e-
CD3OH	CD3OH+	e-
CH2	CH2+	e-
CH2CO	CH2CO+	e-
CH2D	CH2D+	e-
CH2DOD	CH2DOD+	e-
CH2DOH	CH2DOH+	e-
CH3	CH3+	e-
CH3CHD	C2H4D+	e-
CH3CHO	CH3CHO+	e-
CH3CN	CH3CN+	e-
CH3NC	CH3NC+	e-
CH3NH2	CH3NH2+	e-
CH3OCH3	CH3OCH3+	e-
CH3OD	CH3OD+	e-

The main reaction file looks like this:

8 x [8 character] blocks  
First 3 are reactants,  
Last 5 are products;  
photons/CRs are NOT shown.

The three main numbers after the reaction are either the modified Arrhenius coefficients, or other coefficients related to cosmic-ray or photon processes.

The column of "1"s indicates the "ITYPE" of the reaction – the index given to each class of reaction in these networks.

3.52E+02	0.00E+00	0.00E+00	1	1	*	1*
1.76E+02	0.00E+00	0.00E+00	1	2	*	2*
1.02E+03	0.00E+00	0.00E+00	1	3	*	3*
1.31E+03	0.00E+00	0.00E+00	1	4	*	4*
5.00E+02	0.00E+00	0.00E+00	1	5	*	5*
7.78E+02	0.00E+00	0.00E+00	1	6	*	6*
7.80E+02	0.00E+00	0.00E+00	1	7	*	7*
7.78E+02	0.00E+00	0.00E+00	1	8	*	8*
2.74E+03	0.00E+00	0.00E+00	1	9	*	9*
2.62E+03	0.00E+00	0.00E+00	1	10	*	10*
1.06E+04	0.00E+00	0.00E+00	1	11	*	11*
5.30E+03	0.00E+00	0.00E+00	1	12	*	12*
1.12E+03	0.00E+00	0.00E+00	1	13	*	13*
2.24E+03	0.00E+00	0.00E+00	1	14	*	14*
5.00E+02	0.00E+00	0.00E+00	1	15	*	15*
2.87E+03	0.00E+00	0.00E+00	1	16	*	16*
2.87E+03	0.00E+00	0.00E+00	1	17	*	17*
5.00E+02	0.00E+00	0.00E+00	1	18	*	18*
1.22E+03	0.00E+00	0.00E+00	1	19	*	19*
5.00E+02	0.00E+00	0.00E+00	1	20	*	20*
2.87E+03	0.00E+00	0.00E+00	1	21	*	21*
2.87E+03	0.00E+00	0.00E+00	1	22	*	22*
5.00E+02	0.00E+00	0.00E+00	1	23	*	23*
7.78E+02	0.00E+00	0.00E+00	1	24	*	24*
1.12E+03	0.00E+00	0.00E+00	1	25	*	25*
2.24E+03	0.00E+00	0.00E+00	1	26	*	26*
2.24E+03	0.00E+00	0.00E+00	1	27	*	27*
1.12E+03	0.00E+00	0.00E+00	1	28	*	28*
1.12E+03	0.00E+00	0.00E+00	1	29	*	29*
2.87E+03	0.00E+00	0.00E+00	1	30	*	30*

# Chemical networks (OSU, TRICKS, etc.)

The network consists of groupings of various types of reaction. In the OSU and related networks, these are:

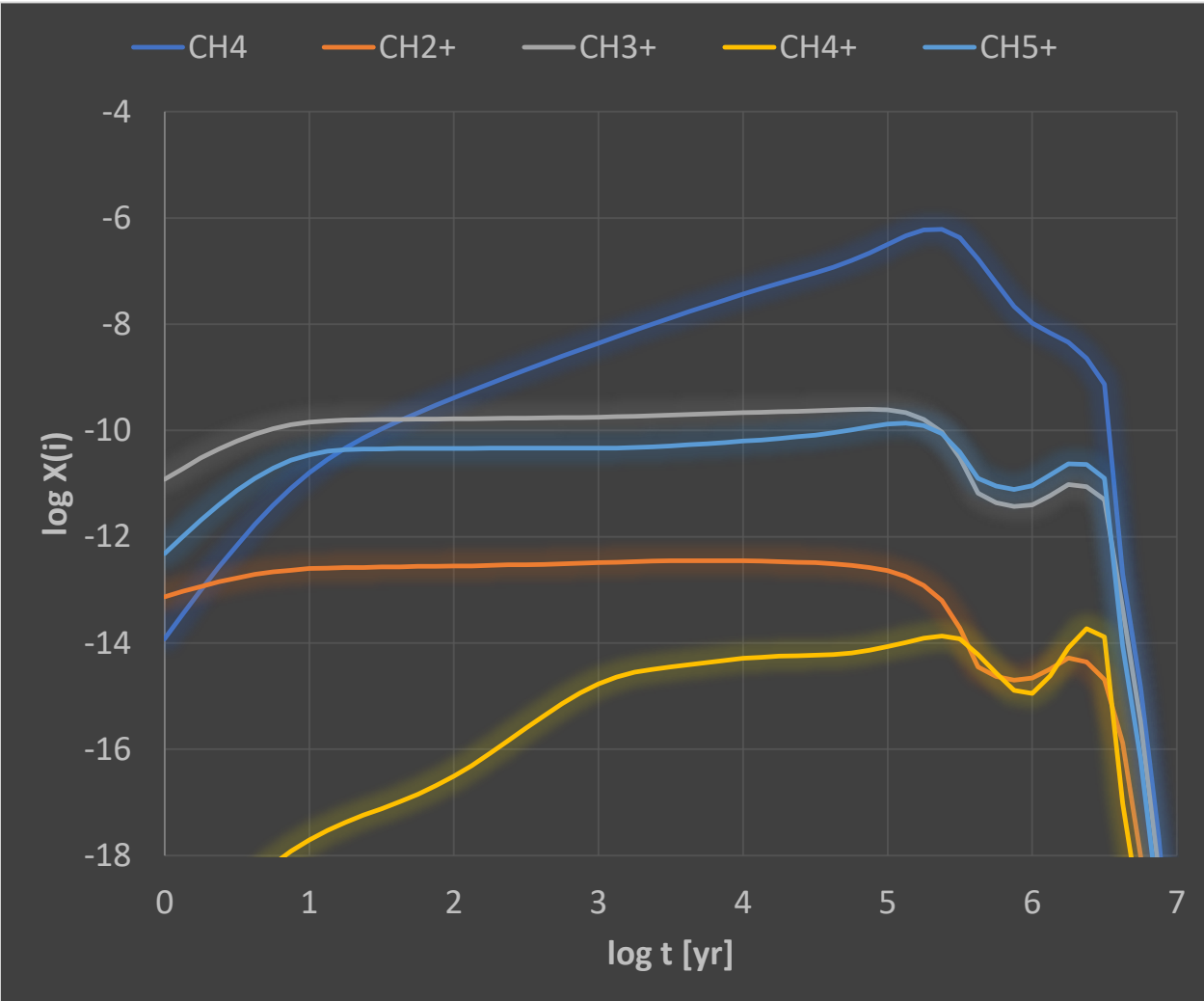
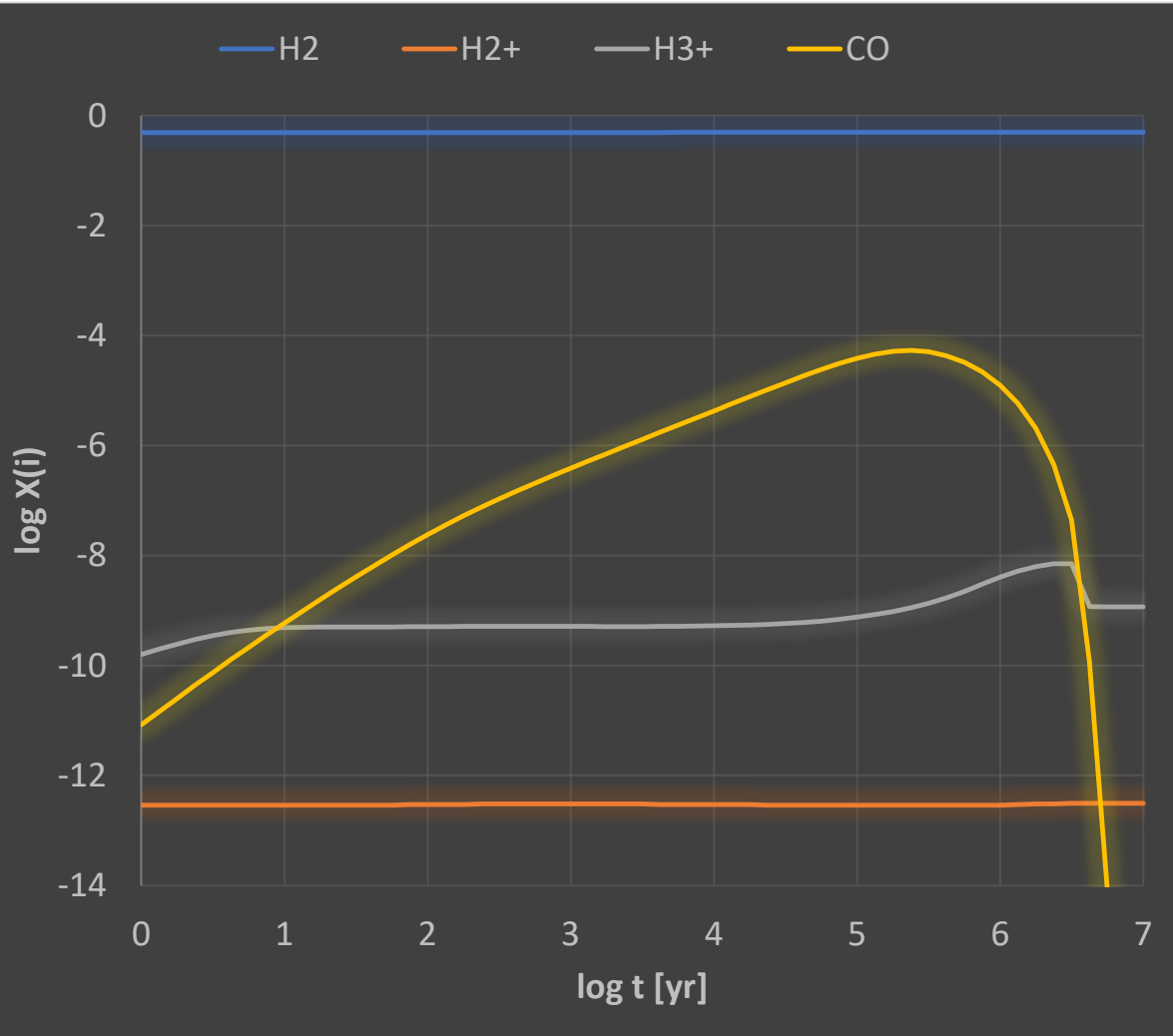
## ITYPE:

- 1) Cosmic-ray induced ionization / dissociation
- 2) Charge-transfer & ion-molecule (most reactions)
- 3) Negative charge transfer
- 4) Radiative association
- 5) Negative ion-neutral
- 6) Chemi-ionization (1 reaction:  $O + CH \rightarrow HCO^+ + e^-$ )
- 7) Neutral exchange
- 8) Neutral radiative association
- 9) Dissociative recombination
- 10) Radiative recombination
- 11) Ion-ion neutralization
- 12) Electron attachment (radiative)
- 13) Photo-ionization/-dissociation

# Output files

- These all have the prefix “top\_” indicating “TRICKS Out Put”.
- There is a main output file, “top\_output.d” that contains the time-dependent fractional abundances of each species. It is an ascii file.
- You could write (e.g.) a Python script to read the abundances, so that you can plot them.
- You could also load one of the “.csv” files directly into a spreadsheet and plot them there. The one labeled “top\_log-log.csv” gives the logarithms of the abundance and time information, to make it easier to plot immediately in a spreadsheet.

You can make plots like these pretty easily in a spreadsheet...



# Order file

- The “order” file, “top\_order.d”, shows the most important formation and destruction processes for each species, at each output time in the model.
- Only reactions contributing to >0.5% of formation or destruction for the species of interest are shown. Less important reactions are not shown. They might be important for other species destroyed or produced by the reaction, though! Check the entries for those species as well!
- It is a pretty big file, so you may want to open it in a bare-bones editor like vi / vim. Window-based editors may seize-up.
- The order file is what really tells you what chemistry is going on.
- It takes a bit of practice to understand, but is very useful.

# Order file

Species number

Chemical species of interest

Its current frac. abundance

Output time index (iteration)

Time in model (yr)

Physical conditions

```

84 >CH      XN= 8.926E-009, IT= 40, t= 5.623E+04 yr, D= 2.000E+04, Av= 10.000, Tg= 10.000
          FORM RATE (s-1)  DEST RATE (s-1)
*11885* H      CH2  --> CH      H2      90%  7.318E-018
*12288* O      C2H  --> CO      CH       3%  2.235E-019
*13138* CH3+   e-    --> CH      H        2%  1.626E-019
*13139* CH3+   e-    --> CH      H2       2%  1.423E-019
*12710* C2H2+  e-    --> CH      CH       1%  9.346E-020
*13453* HCS+   e-    --> CH      S        0%  3.073E-020
*12342* O      CH   --> CO      H       -36% -2.903E-018
*12153* N      CH   --> CN      H       -27% -2.187E-018
*11884* H      CH   --> C        H2      -17% -1.407E-018
*11351* C      CH   --> C2       H       -12% -1.002E-018
*11294* O      CH   --> HCO+    e-      -2%  -1.969E-019
*11514* CH     C3   --> C4       H       -2%  -1.589E-019
* 561* C+     CH   --> C2+    H       -1%  -8.543E-020
* 562* C+     CH   --> CH+    C       -1%  -8.543E-020
          Net production rate  Total formation rate  Total destruction rate
          -9.851E-022         8.109E-018         -8.110E-018

85 >CH2     XN= 1.275E-009, IT= 40, t= 5.623E+04 yr, D= 2.000E+04, Av= 10.000, Tg= 10.000
          FORM RATE (s-1)  DEST RATE (s-1)
*12678* C      H2   --> CH2     H       93%  8.509E-018
*13140* CH3+   e-    --> CH2     H        4%  4.065E-019
* 4587* CH5+   O     --> H3O+   CH2     1%  1.107E-019
*13243* CH5+   e-    --> CH2     H2      0%  4.262E-020
*12806* C3H2+  e-    --> C2     CH2     0%  2.084E-020
*12745* C2H4+  e-    --> CH2     CH2     0%  2.074E-020
*11885* H      CH2  --> CH      H2     -80% -7.318E-018
*12343* O      CH2  --> CO      H        8%  -7.536E-019
*12344* O      CH2  --> CO      H2     -5%  -5.024E-019
*11578* CH2    O     --> HCO    H        3%  -3.146E-019
*11352* C      CH2  --> C2H    H        2%  -2.171E-019
*12154* N      CH2  --> HCN    H        0%  -3.100E-020
          1.448E-023         9.175E-018         -9.175E-018
    
```

Rates of individual formation reactions

Approx. contribution to total formation rate

Net production rate

Total formation rate

Rates of individual destruction reactions

Total destruction rate

Each reaction listed contributes either to the formation or the destruction of the species in question.

Formation reactions are listed first, then destruction.

# “Control file”

- The “control file”, `trx_control.d`, is where you might want to make changes to control the physical conditions of the model, or the initial abundances. The TRICKS code reads this information at run-time. Keep the format the same if you change any quantities.

```
tricks.f vers. 1, trx_control.d: (c) R T Garrod, 2021-
```

---

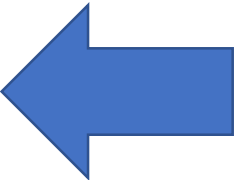
```
SWITCHES
```

IDUST		2		no adsorption (0); allow adsorption (1); adsorption and H reactions (2)
ISELF		1		self-shielding from tables (1): use CDs below; PD rates of H2 & CO in ratefile are replaced
ITASK		1		integrator method for reaching o/p time: exact (3); interp (1)

---

```
GAS PHASE PARAMETERS
```

DENS		2.000D+04		initial gas density (total H per cm <sup>3</sup> )
TEMP		1.000D+01		initial gas temp (K)
AV		1.00D+01		initial visual extinction (mag)
CDH2		8.00D+21		initial H2 column density (cm <sup>-2</sup> )
CDCO		1.00D+18		initial CO column density (cm <sup>-2</sup> )
ZETA		1.300D-17		cosmic ray ionisation rate (s <sup>-1</sup> )
UVFAC		1.000D+00		scale fac for UV radiation field (1=Draine field, i.e. standard)



- It is currently set up to simulate a static dark cloud.
- You can control the physical conditions and a few other things – try it!



# A word of caution about *TRICKS*

- Static models (i.e. fixed physical conditions) like this may be of limited use these days (would have been state-of-the-art 25 years ago).
- Dynamical models are important:  
*How did the initial conditions arise?!*
- The network is:
  - *Quite old*
  - *Mostly limited to gas-phase chemistry*
- *BUT: It is still useful for learning, and testing simple ideas!*

# Thanks for playing!

- Feel free to play with the model as much as you want, for educational purposes.
- The copyright on the code belongs to me, except for the solver (dgear.f).
- Please do NOT upload TRICKS to code-sharing sites/services e.g. Github.
- If you want to TRICKS it for actual research, please let me know – you might prefer a more complete/modern code, but OK.
- If – heaven forbid – you publish something with it, please give attribution to **TRICKS v2.3; (c) R. T. Garrod, 2022**