The Weekly Progress

Since Nov. 10, 2018

In the autumn semester, hopefully I'll record my progress every Thursday morning

Before Nov. 10, 2018

1. Understand why X-ray cause profound effects to ISM

2. Aquire the X-ray spectra emitted the SMBH in the center of Milky Way Galaxy several mys ago

3. Decide to focus on a cold dense cloud 8 kpc from the SMBH, thus fixing the flux

4. Figure out how KROME works, especially its X-ray module (details on https://github.com/slowdivePTG/X-ray-chemistry/tree/master)

5. Be able to calculate primary X-ray ionizations according to a X-ray spectra and the cross sections of certain species.

$$\zeta_k^p = \int_{E_{min}}^{E_{max}} \frac{F_X(E)}{E} \sigma_k(E) \mathrm{d}E$$

$$F_X(E): \ \mathrm{erg} \cdot \mathrm{cm}^{-2} \cdot \mathrm{s}^{-1}$$

6. Learn about the cosmic ray ionization

Nov. 10, 2018

1. Trace the most important reactions using the Jacobian Matrix pd(i,j)

$$pd(i,j) = \frac{\partial}{\partial n(j)} \left(\frac{\mathrm{d}n(i)}{\mathrm{d}t} \right)$$

$$\left(\frac{\mathrm{d}n(i)}{\mathrm{d}t} \right)_j = n(j) \cdot pd(i,j)$$

In `krome_oed.f90`, the `jex` function calculate the Jacobian Matrix.

2. Test a simple model but consider a mixture of H/He rather than H_2/He. $J_{X21} = 0.1$ for 1 mys then turn off the X-ray radiation. Plot the abundance of CH_4 with time.

For this molecular cloud test we choose the **osu_01_2007** network and the initial conditions proposed by *Wakelam & Herbst (2008)*: a constant temperature of $T = 10$ K, H_2 density of 10^4 cm^{-3}, cosmic rays ionization rate of 1.3×10^{-17} s^{-1}, and a visual extinction of 10. The initial conditions of the species are listed in Table 7 and correspond to the EA2 model of *Wakelam & Herbst (2008)*, an high-metal environment observed in the diffuse cloud ζ *Ophiuchi*

```
Tgas = 1d1 !gas temperature (K)
xH = 2d4 !Hydrogen density

!user commons for opacity and CR rate
call krome_set_user_av(1d1) !opacity Av (#)E11.3,
call krome_set_user_crate(1.3d-17) !CR rate (1/s)
call krome_set_user_gas_dust_ratio(7.57d11) !gas/dust

call krome_init()
j21xs = 0d0
call krome_set_J21xray(j21xs)
print *,"J21 Xray = ",j21xs

x(:) = 1.d-20
!initial densities (model EA2 Wakelam+Herbst 2008)
x(KROME_idx_H2)  = 0.5d0   * xH !In this case we actually use
x(KROME_idx_H)   = 0.5d0   * xH, which is not true
x(KROME_idx_He)  = 9d-2    * xH
x(KROME_idx_N)   = 7.6d-5  * xH
x(KROME_idx_O)   = 2.56d-4 * xH
x(KROME_idx_Cj)  = 1.2d-4  * xH
x(KROME_idx_Sj)  = 1.5d-5  * xH
x(KROME_idx_Sij) = 1.7d-6  * xH
x(KROME_idx_Fej) = 2d-7    * xH
x(KROME_idx_Naj) = 2d-7    * xH
x(KROME_idx_Mgj) = 2.4d-6  * xH
x(KROME_idx_Clj) = 1.8d-7  * xH
x(KROME_idx_Pj)  = 1.17d-7 * xH
x(KROME_idx_Fj)  = 1.8d-8  * xH

!calculate elctrons (neutral cloud)
x(KROME_idx_e) = krome_get_electrons(x(:))
```

Nov. 15, 2018

1. (From Prof. Du) The secondary ionization rate of molecular hydrogen can be approximately considered as 2 hydrogen atoms.

> Related readings:
>
> *X-ray chemistry in the envelopes around young stellar objects*, Stäuber 2005
>
> *X-Ray--irradiated Molecular Gas. I. Physical Processes and General Results*, Maloney 1996

According to Maloney 1996, the main process in the X-ray (secondary) ionization of H_2 is:

$$H_2 + e^- \longrightarrow H_2^+ + 2\,e^-$$

We can assume the rate coefficient is twice the ionization rates of H, and thus include it in the network.

> **INCLUDE** means when calculating the secondary ionization rates, we take the abundance of H :

$$n_t(H) = n(H) + 2n(H_2)$$

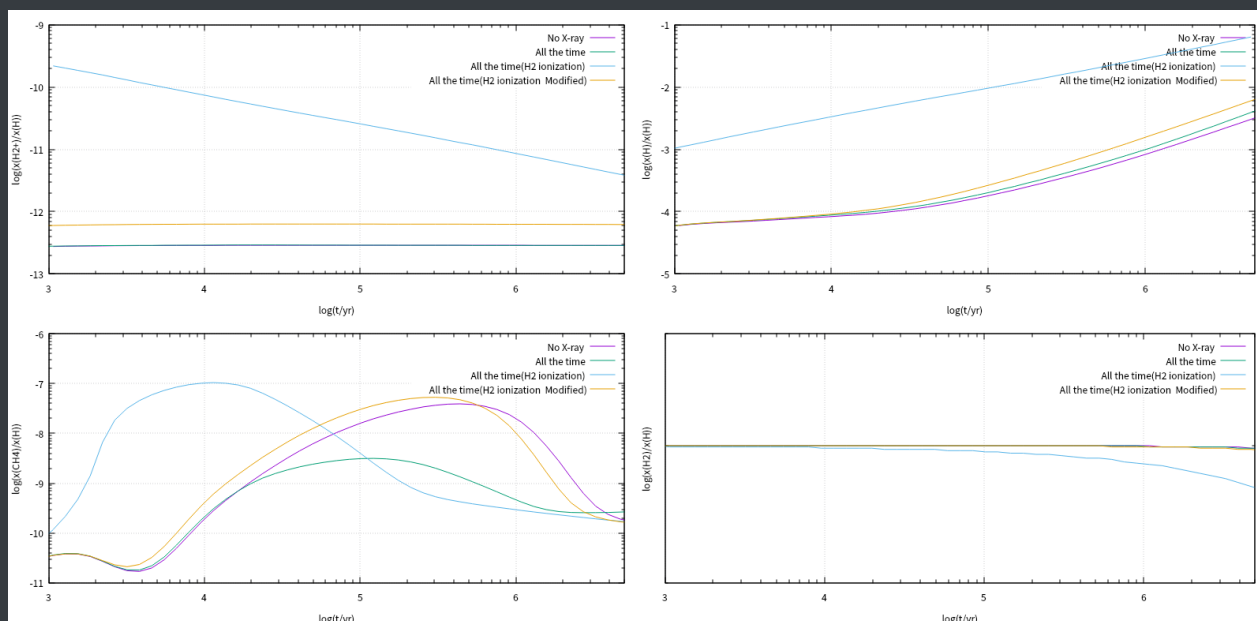The modification of Fortran code in `krome_subs.f90` is shown here

```fortran
!H2 -> H2+ + E
k(38) = rateEvaluateOnce(38)


!H -> H+ + E
k(4430) = small + ((ratexH &
    * (1d0+phiH) + n(idx_He)&
    /(n(idx_H)+2*n(idx_H2)+1d-40) * ratexHe * phiH)&
    * J21xray)

k(38) = k(38) + 2*k(4430)


!HE -> HE+ + E
k(4431) = small + ((ratexHe &
    * (1d0+phiHe) + (n(idx_H)+2*n(idx_H2))&
    /(n(idx_He)+1d-40) * ratexH * phiHe)&
    * J21xray)
```

Some results are:

Obviously the ionization of H_2 becomes more significant, and the profile of CH_4 changes a lot. If we don't take $n_t(H)$ the effect is even more profound.

- *(NOT AT PRESENT)* For heavier atoms or other molecules, we can apply the approximation with the energy E fixed, neglecting the dependence of the cross sections on energy:

$$\zeta_i = \zeta_{H_2} \frac{\sigma_i(E)}{\sigma_{H_2}(E)}$$

2. Species observants most interested in:

> 经常观测的分子包括CO、HCO^+、N_2H^+、HCN、各种碳氢化合物C_2H、C_3H_3等等。可以关注一下代表了电离度的电子丰度x_e，以及H_3^+、C^+、OH^+、H_2O^+等离子的丰度；OH、CH、NH_3、H_2O等也可以看看。还可以看更复杂一些的CH_3CN、CH_3OH等

x_e is important because it decides the chemical composition and whether the heating process is sufficient

3. The simple H/He model used before:

  - Abundance of CH_4 too low
  - Not enough time to form H_2
  - Does not include H_2 formation on **grains**

Therefore it is not reasonable enough, and I shall focus on the new H_2/He model to see what will happen if I turn off the X-ray after 1 mys.

Without H_2 formation on **grains**, there seems no jump in the abundance of CH_4 , which is shown in the plot.
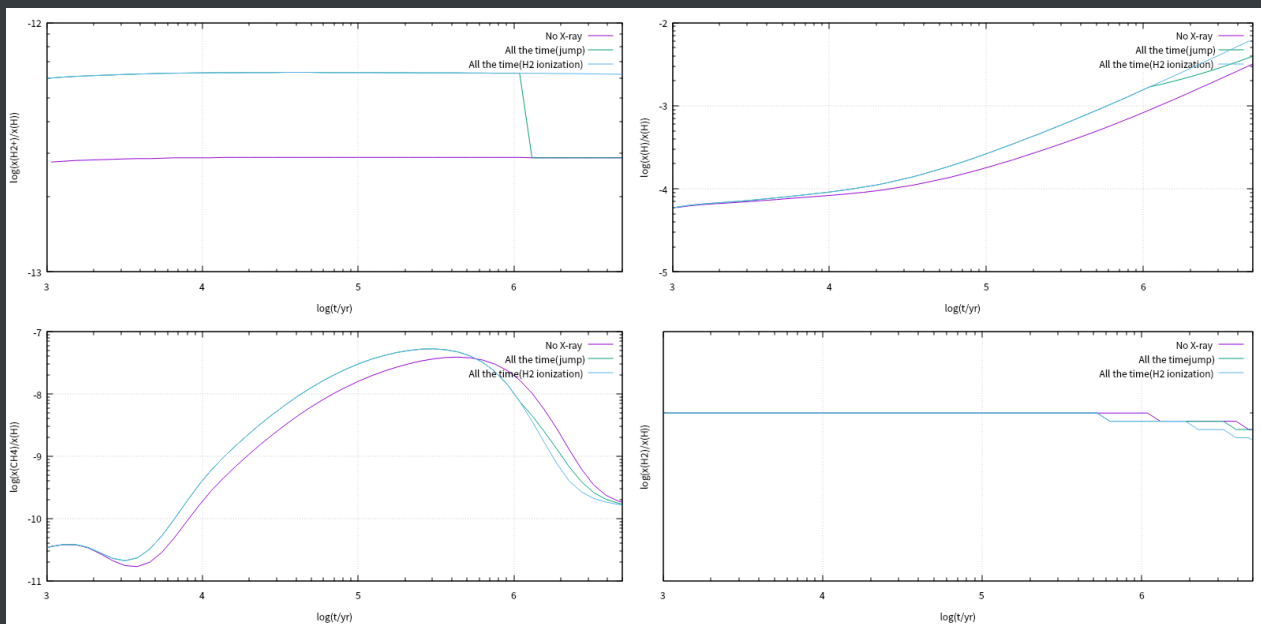
Nov. 22, 2018

1. More details on secondary ionization

   The secondary ionization rate for H (Stäuber 2005, Maloney 1996,):

   $$\zeta_H^{(2)} = \int_{E_{min}}^{E_{max}} \frac{F(E)}{E} N_{sec}(E, x_e)\sigma(E)\mathrm{d}E$$

   $$N_{sec}(E, x_e) = \frac{E - E_{th}}{W(E)} \approx \frac{E}{W(E)}$$

   $N_{sec}(E)$ is the number of secondary **ionizations** per unit energy produced by primary photoelectrons $W(E)$ is the mean energy expended to produce an ion pair through rapid electron process

   A BIG MISTAKE HERE LAST WEEK!

   $N_{sec}(E)$ is not the number of secondary electrons but the number of ion pairs produced by a secondary electron. **WE DON'T COUNT ELECTRONS HERE!**

   More comments on the formula

   - $W(E)$ is nearly independent of E if $E > 200 \ \mathrm{eV}$, which is easy to satisfied in our case
   - $N_{sec}(E, x_e)$ is dependent on x_e. When $x_e > 1\%$, the energy in photoelectrons will be mainly lost to Coulomb Interaction with ambient thermal electrons. In our case, $n_e/n_H < 10^{-4}$. For weakly ionized gases, $\approx 40\%$ of the primary electron energy will be used for ionization (Krolik 1983, Shull 1985) , then for a secondary electron with energy $1 \ \mathrm{keV}$, the number of H it can ionize is:

$$N = \frac{0.40 \times 1\ \mathrm{keV}}{13.6\ \mathrm{eV}} \approx 30$$

More precise calculation (Glassgold & Langer 1973, Dalgarno 1999, Glassgold 2012) shows that in $H_2 + He$ neutral gas, 47% of energy goes to ionization, 47% in H_2 and He excitation, the rest goes for heating. $N_{sec}(E) \approx 27$ and thus we can take $W(E) \approx 37$ eV.

The formula I actually use

$$\zeta_{\mathrm{tot}}^i = \zeta_{\mathrm{p}}^i + \sum_{j=\mathrm{H,He}} \frac{n_j}{n_i} \zeta_{\mathrm{p}}^j \langle \phi^i \rangle$$

- The numbers of secondary ionization of H and He per primary ionization are taken from Shull 1985

$$\phi^{\mathrm{H}}(E, x_{\mathrm{e}}) = \left(\frac{E}{13.6\mathrm{eV}} - 1 \right) 0.3908 \left(1 - x_{\mathrm{e}}^{0.4092} \right)^{1.7592}$$

$$\phi^{\mathrm{He}}(E, x_{\mathrm{e}}) = \left(\frac{E}{24.6\mathrm{eV}} - 1 \right) 0.0554 \left(1 - x_{\mathrm{e}}^{0.4014} \right)^{1.660}$$

- Can be rewritten like this:

$$\zeta_{tot}^{\mathrm{H}} = \zeta_p^{\mathrm{H}} \left(1 + \langle \phi^{\mathrm{H}} \rangle \right) + \zeta_p^{\mathrm{He}} \frac{n_{\mathrm{He}}}{n_{\mathrm{H}}} \langle \phi^{\mathrm{H}} \rangle$$

$$\zeta_{tot}^{\mathrm{He}} = \zeta_p^{\mathrm{He}} \left(1 + \langle \phi^{\mathrm{He}} \rangle \right) + \zeta_p^{\mathrm{H}} \frac{n_{\mathrm{H}}}{n_{\mathrm{He}}} \langle \phi^{\mathrm{He}} \rangle$$

which average ϕ over the X-ray spectrum $F(E)$

2. Test all the species listed last week
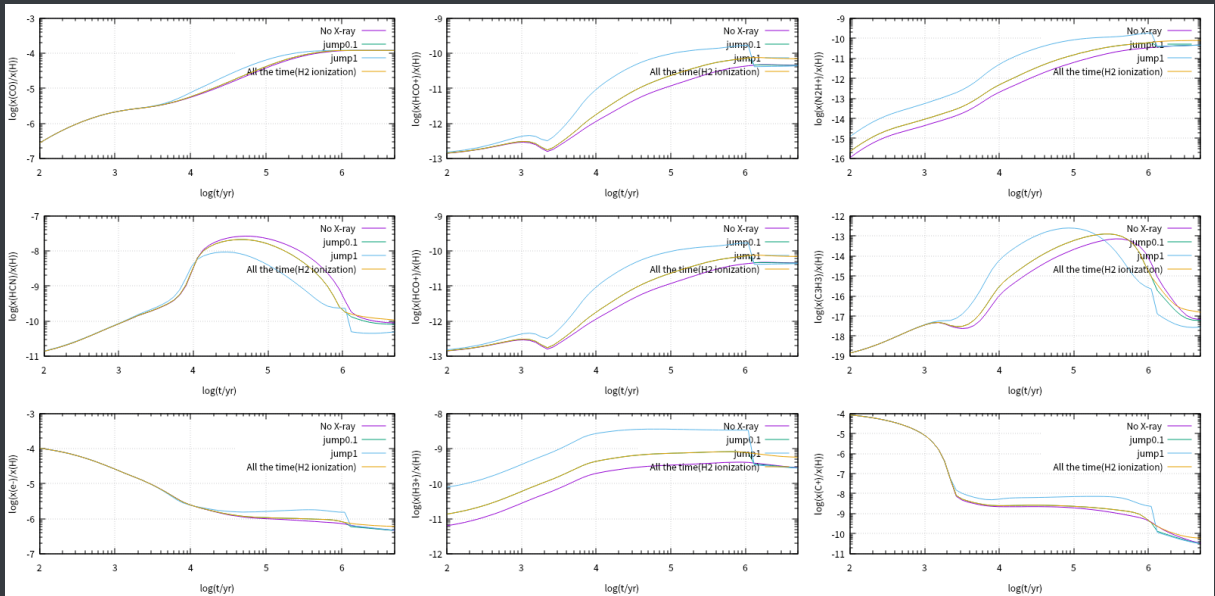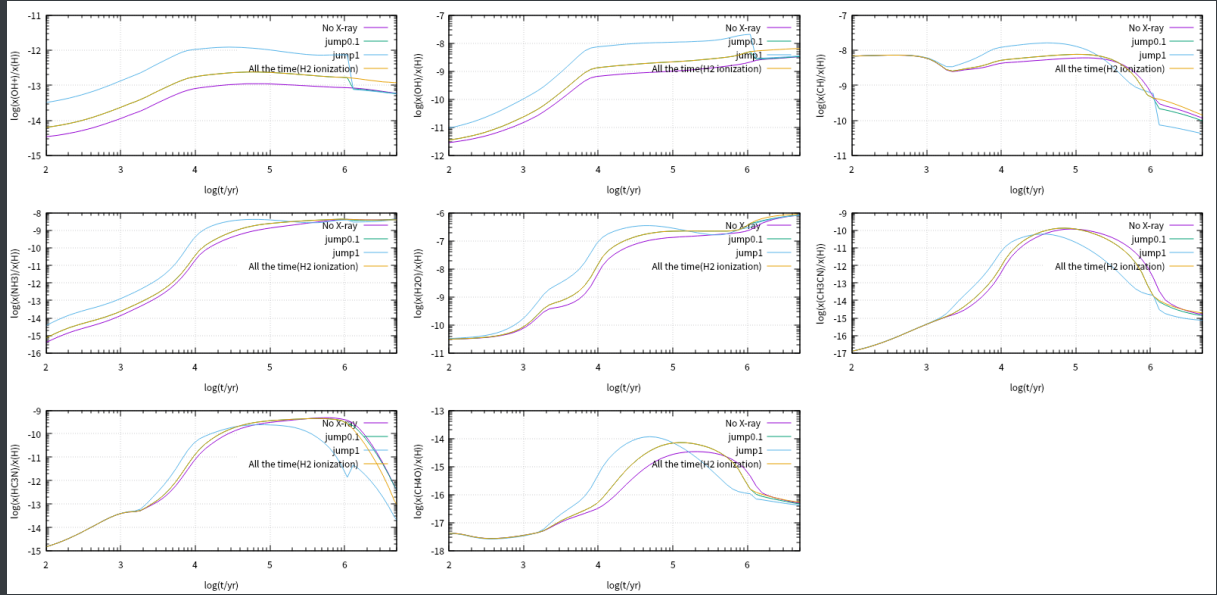
Nov. 29, 2018

1. Recalculate the ionization rate using the primal formula

$$\zeta_{tot}^{\mathrm{H}} = \zeta_p^{\mathrm{H}} + \frac{n_{\mathrm{He}}}{n_{\mathrm{H}}} \int_{E_{min}}^{E_{max}} \frac{F(E)}{E} e^{-\tau(E)} \phi^{\mathrm{H}} \sigma_{\mathrm{He}}(E) \mathrm{d}E + \int_{E_{min}}^{E_{max}} \frac{F(E)}{E} e^{-\tau(E)} \phi^{\mathrm{H}} \sigma_{\mathrm{H}}(E) \mathrm{d}E$$

rather than the simplified one

$$\zeta_{tot}^{\mathrm{H}} = \zeta_p^{\mathrm{H}} \left(1 + \langle \phi^{\mathrm{H}} \rangle\right) + \zeta_p^{\mathrm{He}} \frac{n_{\mathrm{He}}}{n_{\mathrm{H}}} \langle \phi^{\mathrm{H}} \rangle$$

and compare the results.

When we set $n_{\mathrm{H}} = 2 \times 10^4 \ \mathrm{cm}^{-3}, n_{\mathrm{He}} = 2 \times 10^3 \ \mathrm{cm}^{-3}, J_{X21} = 0.1, T = 160 \ \mathrm{K}$, we get

$$\zeta_{\mathrm{H}} = 4.09 \times 10^{-18} \ \mathrm{s}^{-1}, \quad \zeta_{\mathrm{He}} = 3.61 \times 10^{-18} \ \mathrm{s}^{-1} \quad \text{(Primal)}$$

$$\zeta_{\mathrm{H}'} = 7.23 \times 10^{-18} \ \mathrm{s}^{-1}, \quad \zeta_{\mathrm{He}'} = 6.07 \times 10^{-18} \ \mathrm{s}^{-1} \quad \text{(Simplified)}$$

$$\frac{\zeta_{\mathrm{H}}}{\zeta_{\mathrm{H}'}} \approx \frac{\zeta_{\mathrm{He}}}{\zeta_{\mathrm{He}'}} \approx 0.56$$

Since we take $E_{min} = 2 \ \mathrm{keV}, E_{max} = 10 \ \mathrm{keV}$, and in our case, $F(E) \propto E^{-1.5}, \sigma(E) \propto E^{-3}$, $\phi(E, x_e) \propto E, e^{-\tau(E)} \sim 1$, we have

$$\zeta^{(2)} = \int_{E_{min}}^{E_{max}} \frac{F(E)}{E} \phi(E) \sigma(E) \mathrm{d}E = F_0 \phi_0 \sigma_0 \cdot \int_2^{10} E^{-4.5} \mathrm{d}E = \frac{2^{-3.5} - 10^{-3.5}}{3.5} F_0 \phi_0 \sigma_0 \approx 0.025 F_0 \phi_0 \sigma_0$$

and

$$\int_{E_{min}}^{E_{max}} \frac{F(E)}{E}\sigma(E)\mathrm{d}E = F_0\sigma_0 \int_2^{10} E^{-5.5}\mathrm{d}E \approx 0.0098 F_0\sigma_0$$

$$\int_{E_{min}}^{E_{max}} F(E)\phi(E)\mathrm{d}E = F_0\phi_0 \int_2^{10} E^{-0.5}\mathrm{d}E \approx 3.50 F_0\phi_0$$

$$\int_{E_{min}}^{E_{max}} F(E)\mathrm{d}E = F_0 \int_2^{10} E^{-1.5}\mathrm{d}E \approx 0.078 F_0$$

$$\Rightarrow \zeta^{(2)'} \approx \frac{0.0098 F_0\sigma_0 \cdot 3.50 F_0\phi_0}{0.078 F_0} \approx 0.044 F_0\phi_0\sigma_0 \approx 0.57\zeta^{(2)}$$

2. Why does KROME use a simplified formula to calculate the total ionization rate?

- $\zeta_p^{\mathrm{H}}, \zeta_p^{\mathrm{He}}$ are stored in data-files rateH.dat and rateHe.dat (column density *v.s.* primary ionization rate)
- To calculate $\zeta^{(2)}$ the program needs to read $x_e, n_{\mathrm{H}}, n_{\mathrm{He}}$ for each calculation
- By using the simplified formula, we may avoid integration

Here is part of the codes (`krome_subs.f90`):

```
T = Tgas
Trad = 2d4
ncolH = num2col(n(idx_H)+2*n(idx_H2),n(:))
ncolHe = num2col(n(idx_He),n(:)) !number density to column
density
logHe = log10(ncolHe) !take log
logH = log10(ncolH)
xe = min(n(idx_e) / (get_Hnuclei(n(:)) + 1d-40), 1d0)
user_xray_H = fit_anytab2D(user_xray_H_anytabx(:), &
    user_xray_H_anytaby(:), &
    user_xray_H_anytabz(:,:), &
    user_xray_H_anytabxmul, &
    user_xray_H_anytabymul, &
    logH,logHe-logH)
    !linear interpolation to find the proper rate for the column
density
phiH = .3908d0*(1e0-xe**.4092)**1.7592 * 327.832286034056d0 !
avoid integration
ratexH = 1d1**user_xray_H
user_xray_He = fit_anytab2D(user_xray_He_anytabx(:), &
    user_xray_He_anytaby(:), &
    user_xray_He_anytabz(:,:), &
    user_xray_He_anytabxmul, &
    user_xray_He_anytabymul, &
    logH,logHe-logH)
phiHe = .0554d0*(1d0-xe**.4614)**1.666 * 180.793458763612d0
ratexHe = 1d1**user_xray_He
```

```fortran
        k(:) = small !inizialize coefficients

        !H -> H+ + E
        k(1) = small + ((ratexH &
            * (1d0+phiH) + n(idx_He)&
            /(n(idx_H)+1d-40) * ratexHe * phiH)&
            * J21xray)

        !HE -> HE+ + E
        k(2) = small + ((ratexHe &
            * (1d0+phiHe) + n(idx_H)&
            /(n(idx_He)+1d-40) * ratexH * phiHe)&
            * J21xray)

        print '(a10,E15.8)',"XrateH:",log10(k(1))
        print '(a10,E15.8)',"XrateHe:",log10(k(2))
        coe(:) = k(:) !set coefficients to return variable
```

Dec. 5, 2018

1. Try to repeat some results in former papers…but pretty difficult to do

   - Krolik 1983 did not consider the X-ray ionization of H_2

     > Dec. 12 review: Actually, H_2 ionization is considered with an approximate model (Brown and Gould's 1970)

   - Those who have considered the x-ray ionization of H_2 usually have too complex physical problems and models, which means they are not easy to fully understand and repeat within hours
   - The model we consider is simple and does not include heating/cooling process and totally ignore UV-photon process

2. Add molecular hydrogen formation process to the network (from react_primordial, primordial rates from several authors mostly based on Abel et al. 1997 + Grassi et al. 2014)

Dec. 12, 2018

1. Reread and try to repeat the results in Krolik 1983.

   A Review on Krolik 1983

- Modify the codes
  - Initial abundances
  - Longer time period (steady-state solutions) $\Delta t = 10^8$ yrs

    (Strange tendency appears when $\Delta t > 10^8$ yrs, abundances of some species changes rapidly)
  - Set two branches for H_2 ionization & dissociation
  - Add H_2 formation process on grains
- Step 1. Still use the power law spectrum,
  - It is the total ionization rate rather than the detail of the spectrum that is the most important to the chemistry

2. A new paper on the enhanced molecular ionization in the central molecular zone of our Galaxy

   Molecular Ionization Rates and Ultracompact Dark Matter Minihalos, Silk, J. 2018, PRL

Dec. 20, 2018

1. Grain Process
   - It's important to find out how H_2 molecules form on the grain surface as well as how KROME deal with the process
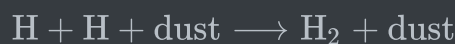
     $$H + H + dust \longrightarrow H_2 + dust$$
   - Theoretically, KROME uses

     $$\frac{dn_{H_2}}{dt} = \frac{\pi}{2} n_H v_g \sum_{j \in [C,Si]} \sum_i n_{ij} a_{ij}^2 \epsilon_j (T, T_i) \alpha (T, T_i)$$

     where v_g is the gas thermal velocity, a_{ij} is the size of the grain, T_i is the dust temperature, ϵ_j depends on the type of the dust and α is the sticking coefficient
   - The rate is defined in the file `krome_dust.f90`

```fortran
function krome_H2_dust(nndust,Tgas,Tdust,nH,H2_eps_f,myvgas)
    !H2 formed on dust (1/cm3/s)
    use krome_constants
    use krome_commons
    real*8::H2_dust, krome_H2_dust,Tgas,Tdust(:)
    real*8::myvgas,H2_eps,nndust(:),nH,H2_eps_f
    integer::i

    H2_dust = 0.d0
    do i = 1,size(Tdust)
       H2_eps = H2_eps_f(Tgas, Tdust(i))
       H2_dust = H2_dust + 0.5d0 * nH * myvgas * nndust(i) &
```

```
              * krome_dust_asize2(i) &
              * pi * H2_eps * stick(Tgas, Tdust(i))
        end do

     krome_H2_dust = H2_dust

   end function krome_H2_dust
```

as well as related functions. Again in `krome_ode.f90` this rate is added to the total rate of H_2 formation. The process is shown in `kromeobj.py` where

```
#add H2 formation on dust
if(self.useDustH2const):
    if("H"==specs[idnw].name): x += " - 2d0*nH2dust"
    if("H2"==specs[idnw].name): x += " + nH2dust"
```

2. Slightly modify the X-ray ionization

   ▪ In Krolik 1983, there are two branches for molecular Hydrogen ionization (See **X-ray** module in the review)

   ▪ Modify the `krome_subs.f90`

```
!H2 -> H+ + H + E
k(36) = rateEvaluateOnce(36)


!H2 -> H2+ + E
k(38) = rateEvaluateOnce(38)


!H -> H+ + E
k(4452) = small + ((ratexH &
    * (1d0+phiH) + n(idx_He)&
    /(n(idx_H)+2*n(idx_H2)+1d-40) * ratexHe * phiH)&
    * J21xray)

!1keV cross section ratio
k(14) = k(14) + 150*k(4452) !C
k(22) = k(22) + 400*k(4452) !O
k(20) = k(20) + 280*k(4452) !N
k(19) = k(19) + 7*k(4452)  !Mg
k(36) = k(36) + 2*k(4452)*0.2
k(38) = k(38) + 2*k(4452)*0.8

!Many molecular species are also included
```

```
!HE -> HE+ + E
    k(4453) = small + ((ratexHe &
        * (1d0+phiHe) + (n(idx_H)+2*n(idx_H2))&
        /(n(idx_He)+1d-40) * ratexH * phiHe)&
        * J21xray)
```
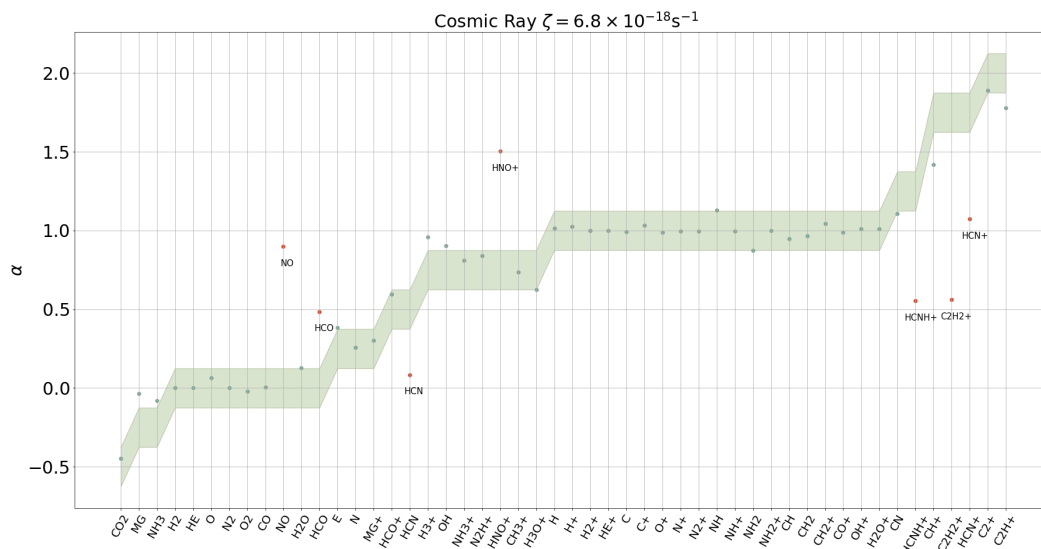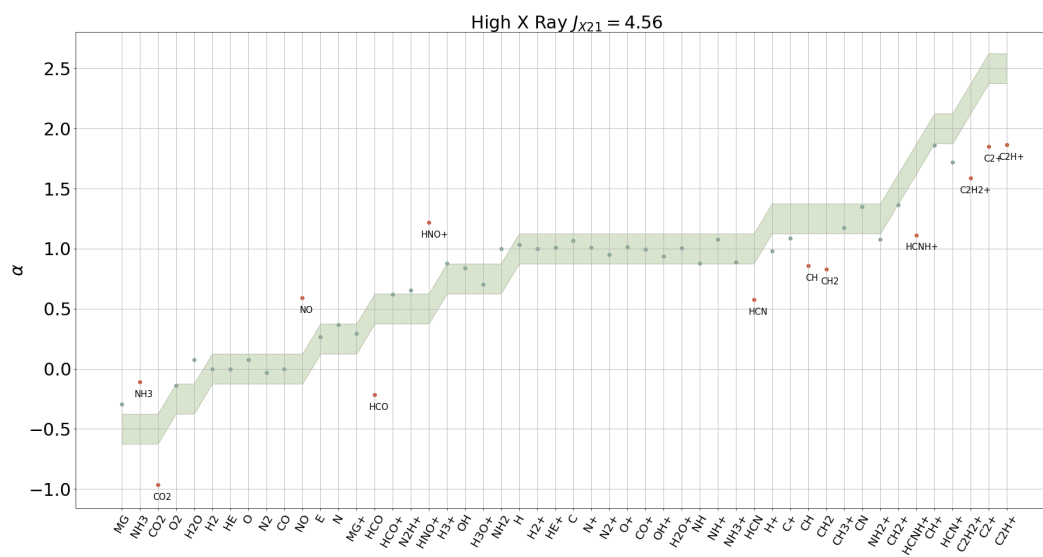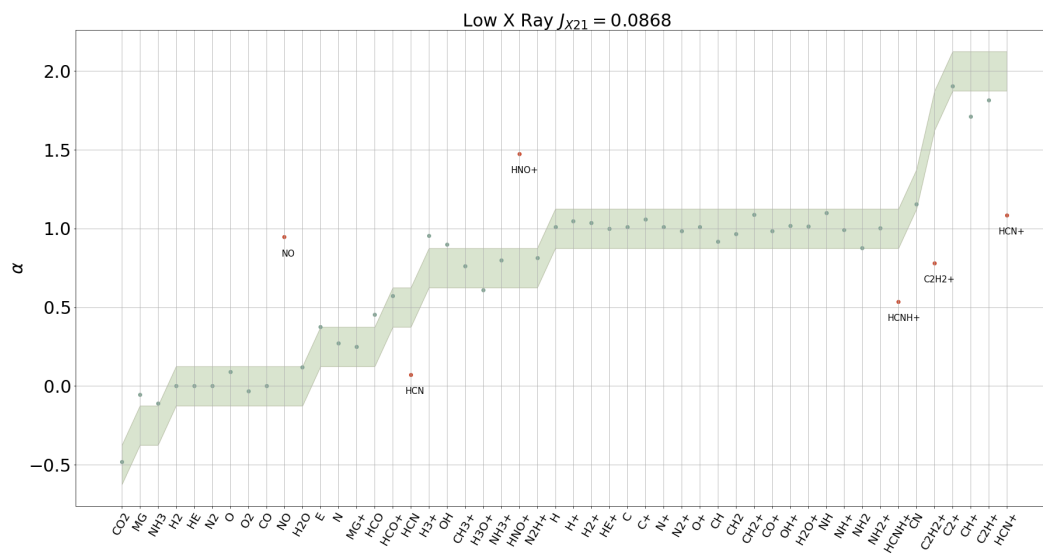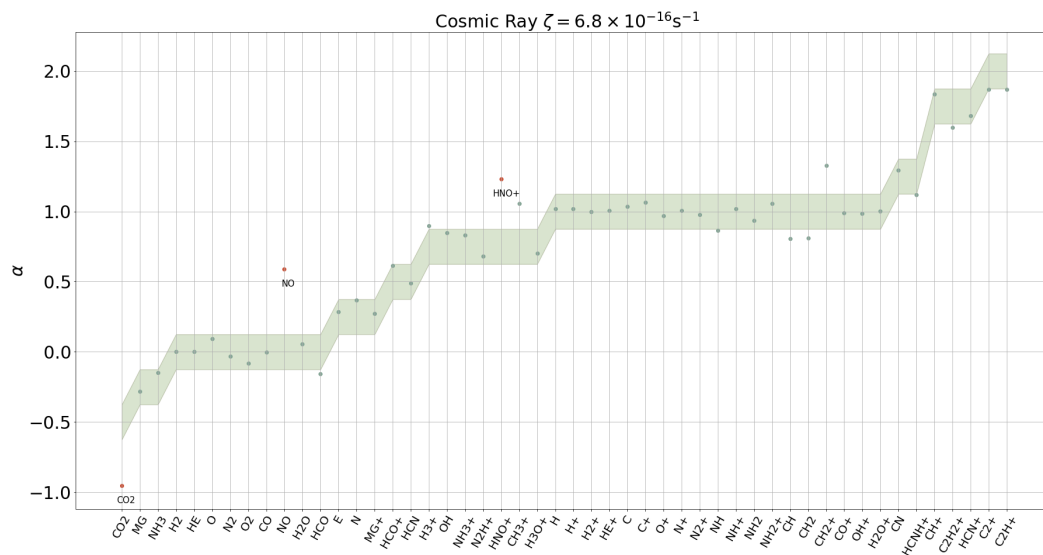
3. Repeat Krolik's results

   ▪ Cosmic ray

      ▪ well matched, except for several species such as HNO^+ which has a larger α.
      ▪ The difference in α between stronger and weaker ionization rates is larger.

   ▪ X-ray

      ▪ For lower ionization rate (Jx21=0.08 and 8), the result is not far from Krolik's.
      ▪ For high ionization rate (Jx21=80), a strange problem occurs at about 20 million yrs, when the abundances of many species and reaction rates change by a few order of magnitude 'in a sudden'. Perhaps because of some calculation errors in the program?
      ▪ There seems not to be a state of chemical equilibrium, the abundance of molecular Hydrogen continue to go down.

4. Ameliorate the program to trace the important species

Dec. 27, 2018

1. Plot and compare the α of Krolik's and the calculation results

Cosmic Ray $\zeta = 6.8 \times 10^{-16} \mathrm{s}^{-1}$

Low X Ray $J_{X21} = 0.0868$

High X Ray $J_{X21} = 4.56$

Jan. 3, 2019

1. Find the internal time-step of KROME to see whether it may cause instability of the calculation.

   In the introduction of KROME, it goes like this

   > Note that the internal time-step of Krome is chosen according to the ODE system and the stiffness of the set of equations is evaluated and the user has no need to provide it, since it is automatically determined by the solver using the values of relative and absolute tolerance employed.

   Do I have to find out how the solver would choose the value?

Jan. 16, 2019

1. Realize that there is a mistake in the rate coefficient of H. The result is that the number of each atom is not conserved so there would not be any equilibrium state for the system. After fixing the bug, the system reaches equilibrium within as most several million years whatever the initial condition is, and we can re-plot the diagram.

   In this case the step-length should be okay, and there seems no threshold of abundances. For safety I set a lower bound of `1d-99*nH` for each species.

2. For high ionization rate situation, the result is far from Krolik's though a steady equilibrium is quickly reached.
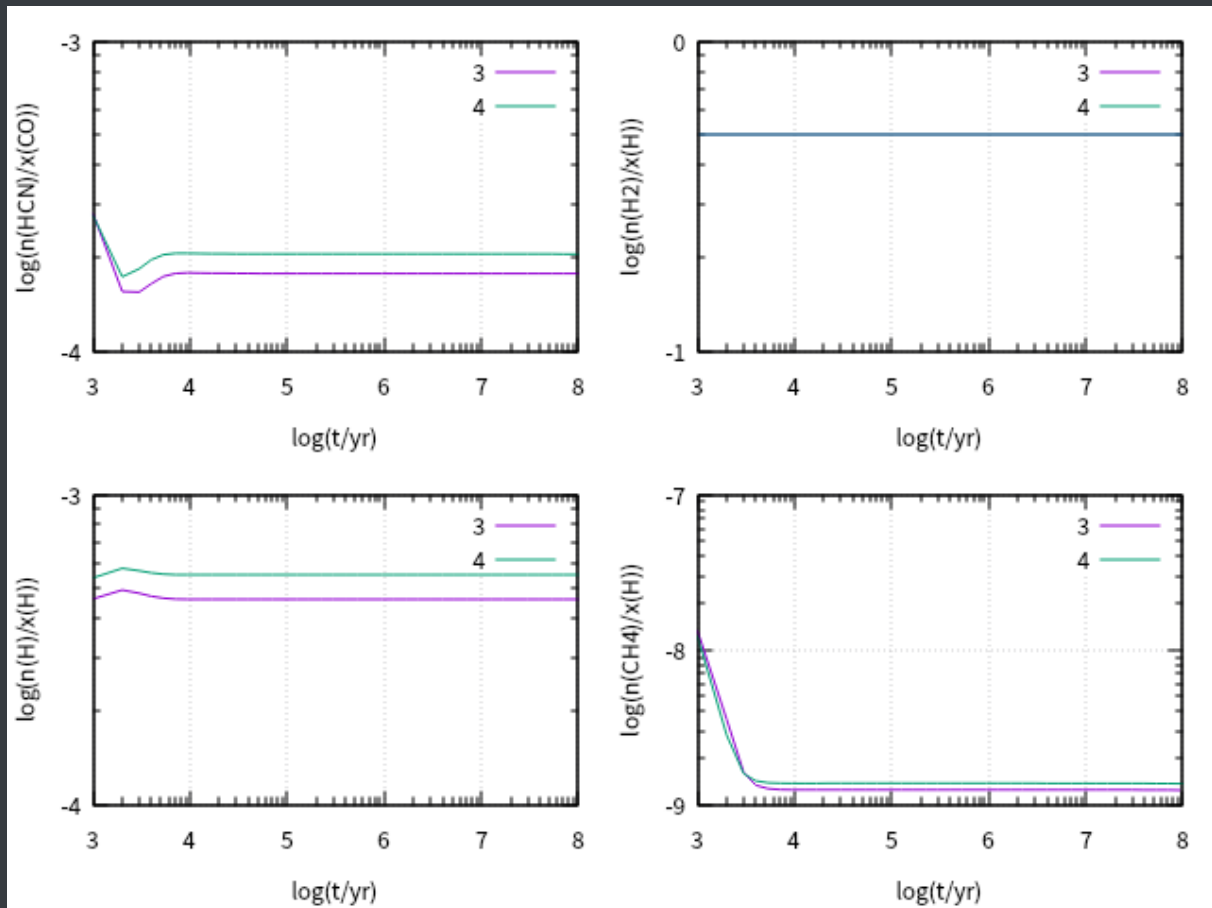
Jan. 24, 2019

1. Recheck the X-ray ionization mechanism in the present code and compare the mechanism with those in present papers.
2. Move on.

Feb. 19, 2019

1. Consider electron cross section ratios in the calculation of secondary ionization of other species according to Maloney+ 1996

In `krome_subs.f90`

```
! 50eV cross section ratio
k(14) = k(14) + 3.1136*k(4452) !C
k(22) = k(22) + 1.5957*k(4452) !O
k(20) = k(20) + 2.0029*k(4452) !N
k(19) = k(19) + 13.1726*k(4452) !Mg
k(36) = k(36) + 2*k(4452)*0.05
k(38) = k(38) + 2*k(4452)*0.95


!C2 -> C + C
k(26) = k(26) + 3.1136*2*k(4452)
```

```
!CN -> C + N
k(30) = k(30) + (2.0029+3.1136)*k(4452)


!CO -> C + O
k(31) = k(31) + (3.1136+1.5957)*k(4452)*0.8


!CO -> CO+ + E
k(32) = k(32) + (3.1136+1.5957)*k(4452)*0.2


!NH -> N + H
k(45) = k(45) + (1+2.0029)*k(4452)


!NO -> N + O
k(46) = k(46) + (2.0029+1.5957)*k(4452)*0.8


!NO -> NO+ + E
k(47) = k(47) + (2.0029+1.5957)*k(4452)*0.2


!O2 -> O + O
k(49) = k(49) + 1.5957*2*k(4452)*0.8


!O2 -> O2+ + E
k(50) =k(50) + 1.5957*2*k(4452)*0.2


!H2O -> OH + H
k(72) = k(72) + (1.5957+2)*k(4452)


!HCN -> CN + H
k(75) = k(75) + (1+3.1136+2.0029)*k(4452)


!HCO -> CO + H
k(76) = k(76) + (1+3.1136+1.5957)*k(4452)*0.8


!HCO -> HCO+ + E
k(77) = k(77) + (1+3.1136+1.5957)*k(4452)*0.2
```

Mar. 2, 2019

1. Include X-ray heating and H_2 cooling processes to the code, still with bugs.

Mar. 14, 2019

1. Got Guangshuai's spectra, writing pipelines to plot and calculate X-ray spectra in different distances from Galactic center and different X-ray models (different α, β, $\dot{m}$)

2. Plot several figures

   - The standard (Latif+ 2015) X-ray spectra in comparison with Guangshuai's data (both with and without absorption)

     - $J_{X21} = 0.1, 1, 10$
     - $\alpha = 0.1, \beta = 100, \dot{m} = 0.5$ in difference distances $(1, 2, 4, 8 \text{ kpc})$
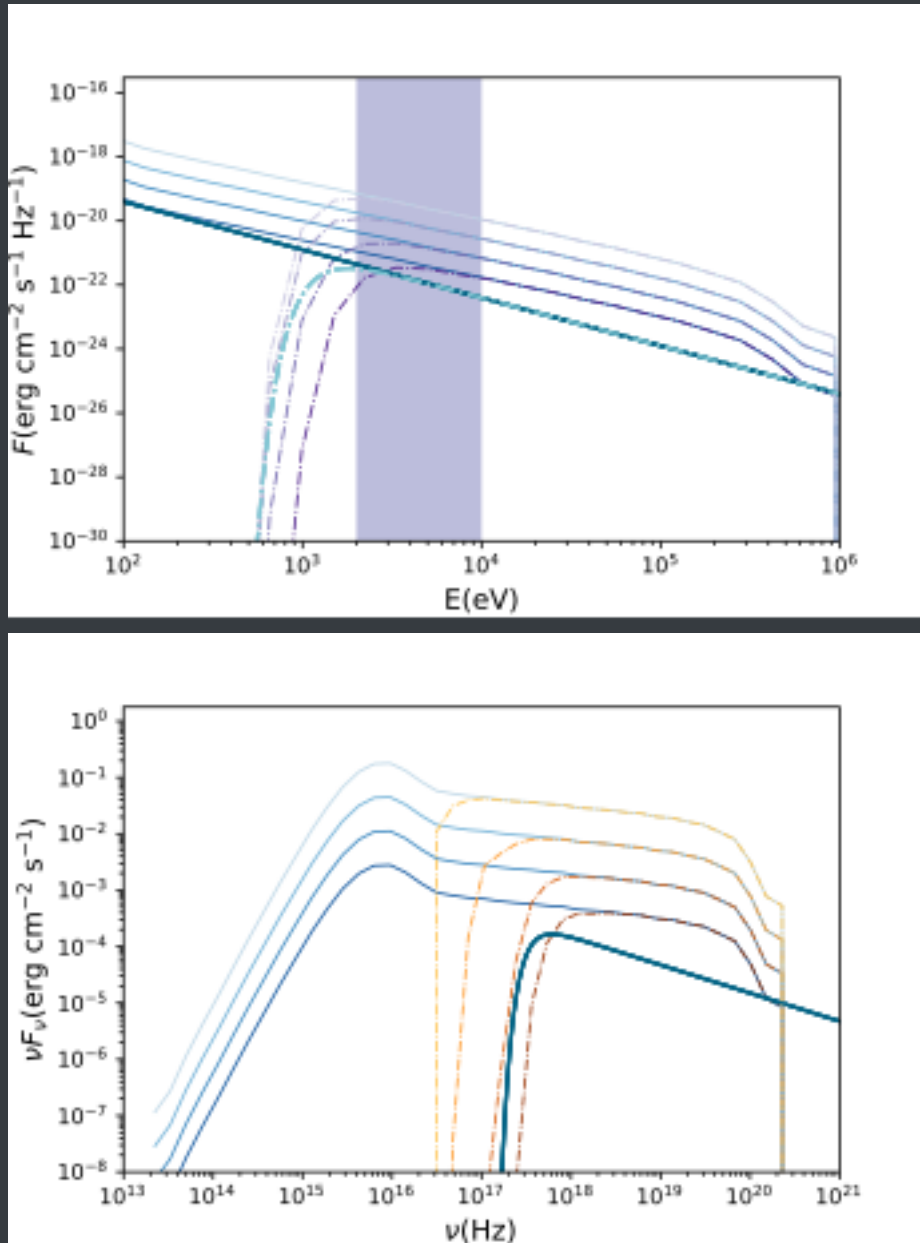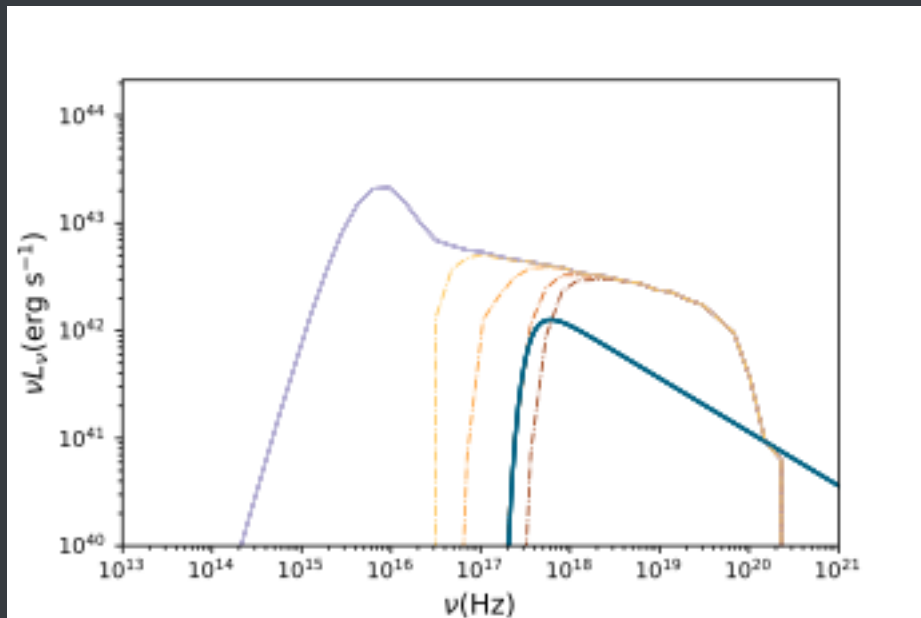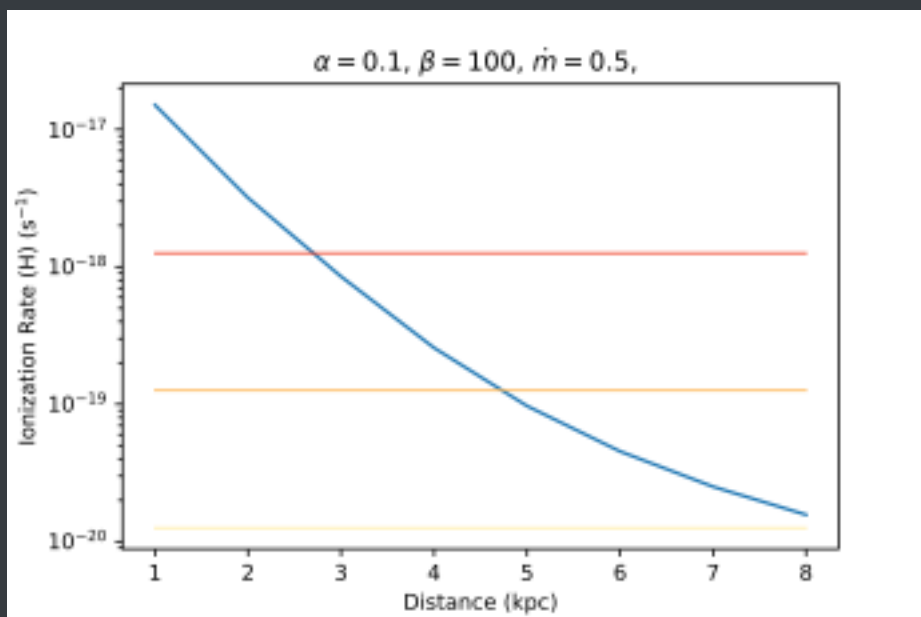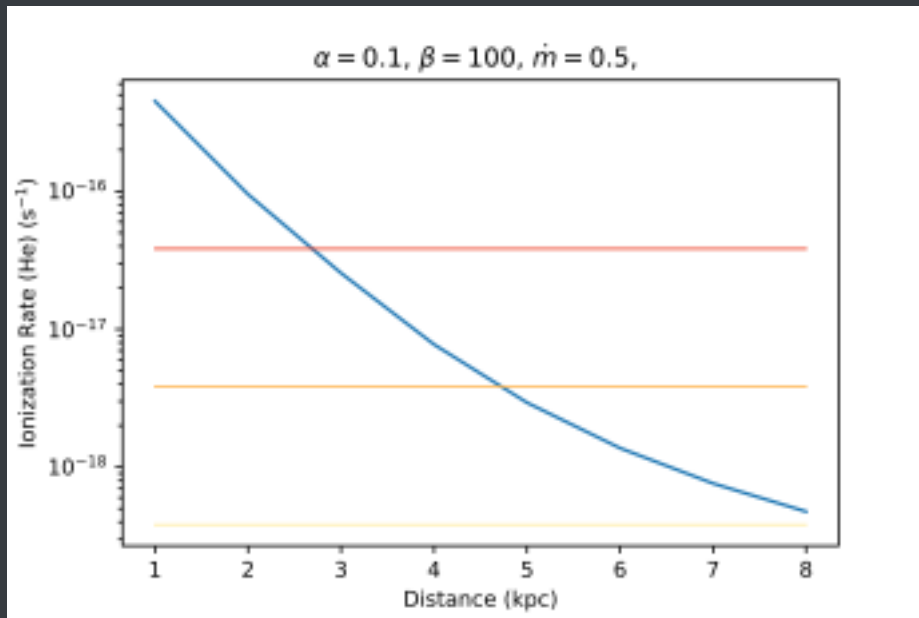
- The total flux in different distances as well as using the standard spectrum

Figure title: $\alpha = 0.1,\ \beta = 100,\ \dot{m} = 0.5,$
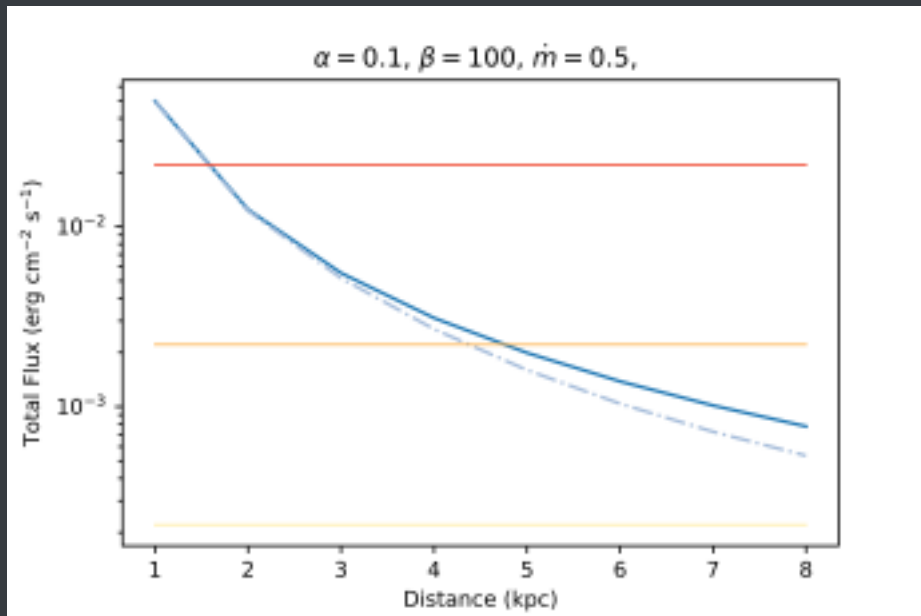
- The comparison in ionization rates

Figure title: $\alpha = 0.1,\ \beta = 100,\ \dot{m} = 0.5,$

$\alpha = 0.1,\ \beta = 100,\ \dot{m} = 0.5,$

Mar. 23, 2019

1. More insights into `ratexH.dat/ratexHe.dat`

   To convert column density to number density, the datafile seems not to use the Jeans length but utilize an approximation to simplify the calculation. Details in `The way KROME calculates the 'auto' ionization rate`

2. Succeed in creating `ratexH.dat` using Guangshuai's data, using Jeans length and formula

$$N^i = n^i \frac{\lambda_j}{2}$$

   for number density/column density conversion

3. Sucessfully repeat the EA1 and EA2 cases in Wakelam & Herbst 2008, which shows the evolution of certain species without X-ray

Mar. 26, 2019

1. Distinguish between the direct ionization of heavy elements and the secondary ionization of heavy elements/molecules due to the fast electrons released mainly by H_2 and He. The former causes Auger effect, which means a K-shell electron will be ionized and an outer electron will fill in the room. To get rid of extra energy the atom release another electron (Auger electron) and is thus doubly ionized. Doubly ionized species will soon react with other molecules or dissociate to form two singly charged parts (for molecules). **However**, as we consider mainly the secondary ionization, we do not count direct ionization of heavy elements and again use the approximation

$$\zeta_m \approx \frac{\sigma_{e,m}(E)}{\sigma_{e,H_2}(E)} \zeta_{H_2}$$

$\sigma_{e,m}$ can be found on NIST (atom) or NIST (molecule)

2. Several possible reasons for the inconsistency with Krolik's work

   - We do not consider directly ionization of heavy elements, neither do we include doubly charged species (according to Maloney+1996 they are usually not important)

   - Our chemical network is much larger

   Eg. NH_3

   NH_3 is included in Krolik's network. In the X-ray ionization case, when the ionization rate $\zeta \approx 7 \times 10^{-16}$, the α value of NH_3 given by Krolik is low as ~ 0.5 , significantly lower than ~ 0 as we calculated. Krolik notes that the destruction of NH_3 is mainly due to the reaction with ionized C^+, however, using the trace module I wrote, I discover that this is not the case. NH_4^+ accounts for the formation of NH_3 and the reaction rate is one order of magnitude higher than the destruction rate due to C^+. As a test, I 'stopped' the reaction below

   $$NH_4^+ + e^- \longrightarrow NH_3$$
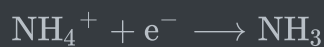
   As a result, the α value of NH_3 is much closer to Krolik's result, which is also true for $\zeta \approx 7 \times 10^{-18}$, suggesting that there may be reactions that Krolik did not consider which influence the sensitivity of some species to the X-ray ionization

Apr. 1, 2019

1. Continue on looking for the differences between the current chemical network and Krolik's network, but have not found any species with significant impacts on the α group as NH_4^+ does. The best simulation result (closest to Krolik's) is
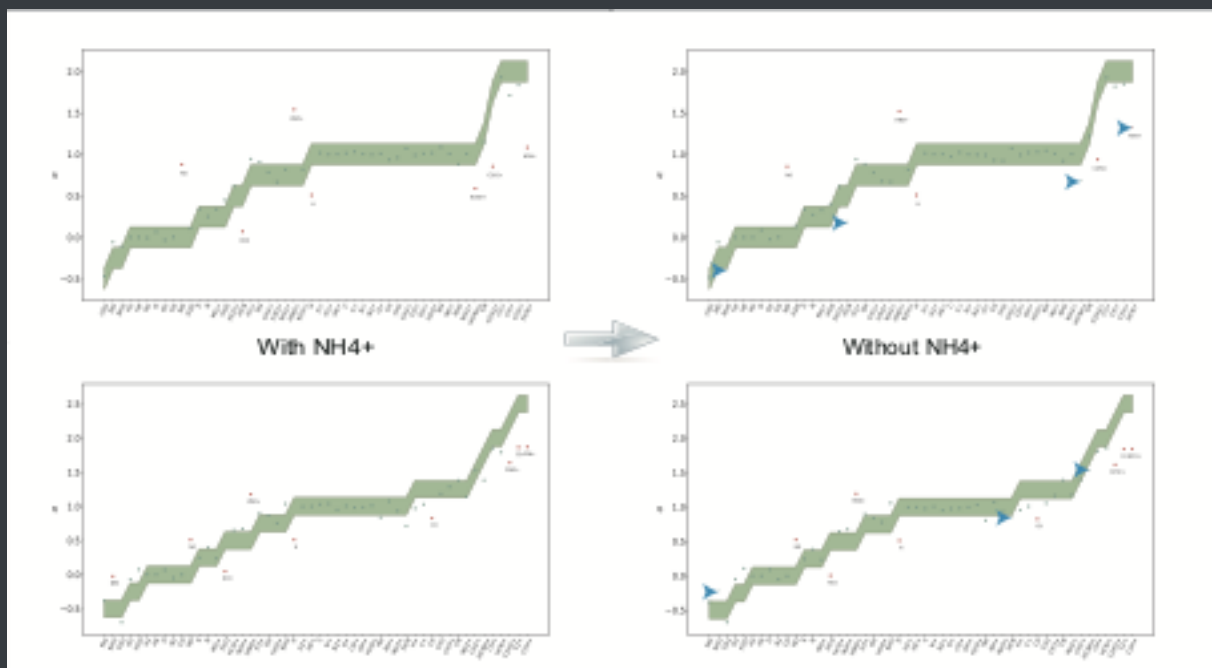
Apr. 7, 2019

1. Review several important molecules that are closely related to observations (details in Observations and Important Molecules)

   - Si/SiO - grain process induced by shocks or X-ray evaporation
   - HCO^+/HOC^+
   - CN/HCN
   - Several species v.s. CO

To do list

1. Check again the consistency with former work
2. Find more physical details of ISM closer to the galactic center with higher temperature and higher degree of ionization.
3. Figure out the extra process we need to consider (such as heating when the degree of ionization is high).