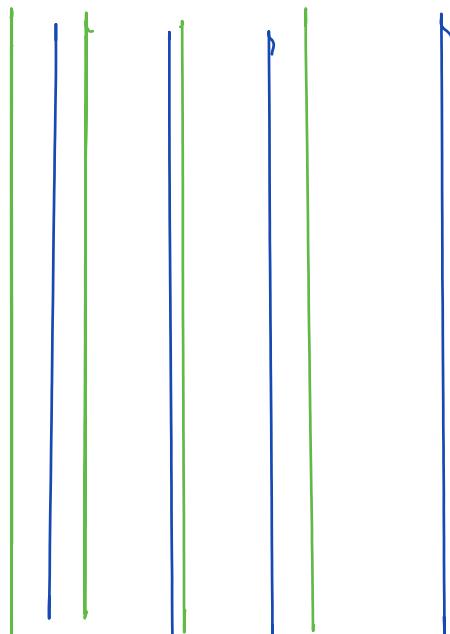


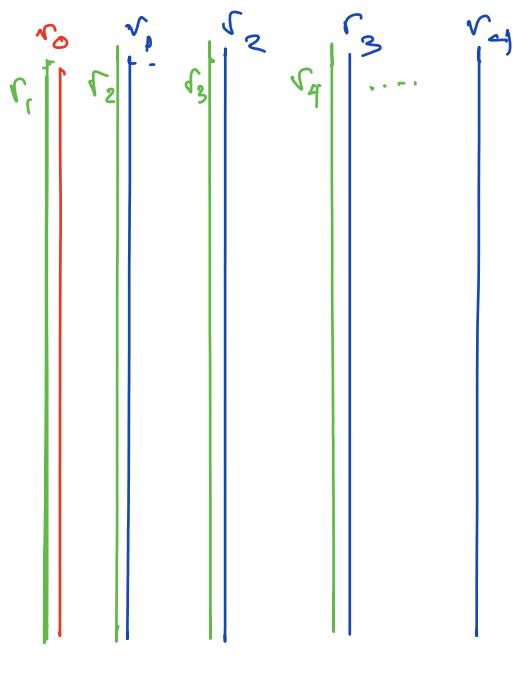
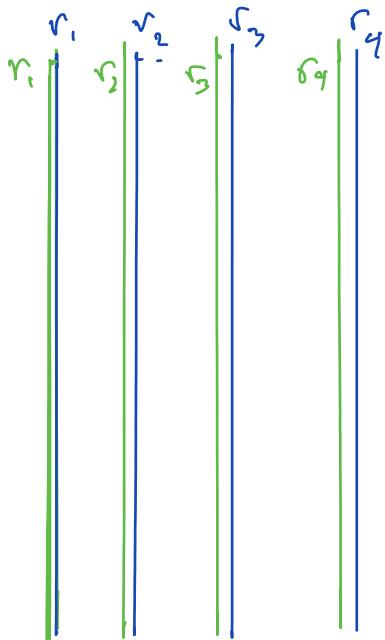
NO^+ ions shells move w/
velocity proportional to r_i
and charge gradient

NO^* neutrals stationary to
first approx, gain vel
by charge transfer



NO^* neutrals

NO^+ ions



Self Similarity
velocity such
that when
shell i advances
to overlap boundary
to shell $i+1$
expansion of
shells cause
all to align

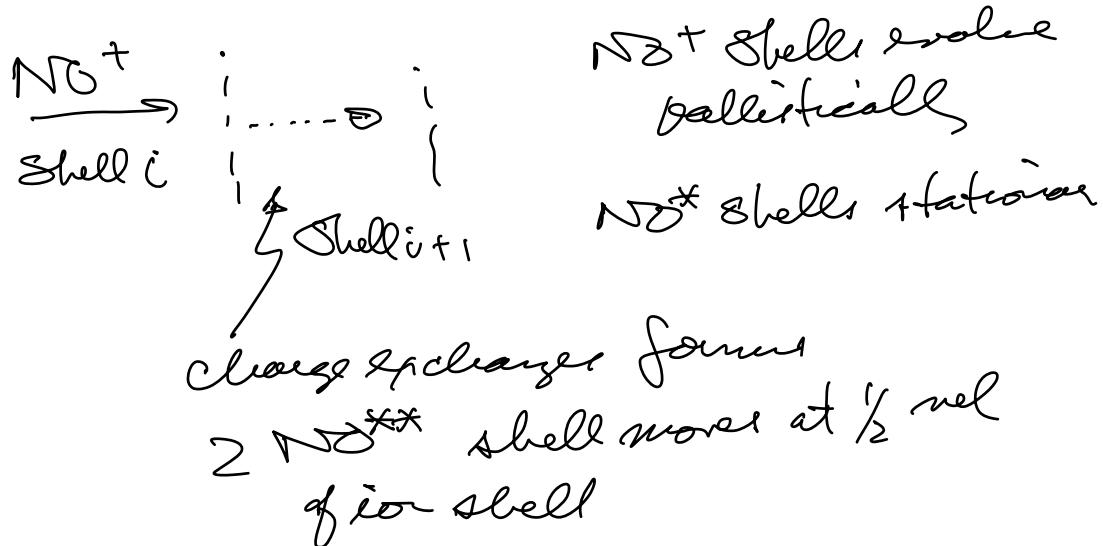
Rule: over the interval t , determine which
shells advance by 1 index number
charge transfer occurs according to
cross section, ρ_{tot} , path length and t

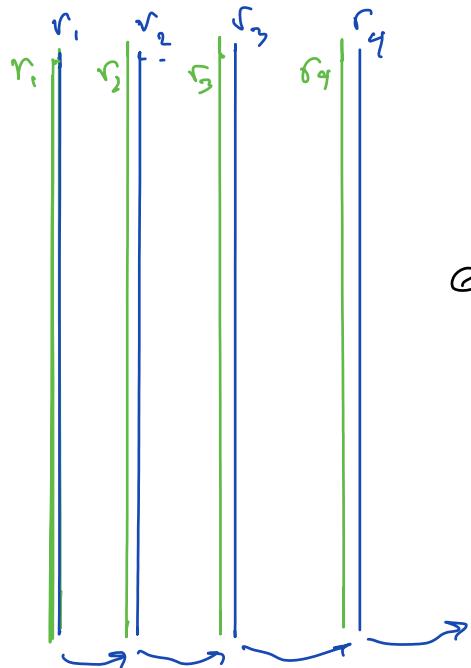
Every charge exchange reaction that occurs within shell i subtracts energy $\frac{1}{2}m\dot{v}_i^2$ from ion shell separation and adds energy $\frac{1}{2}m\dot{v}_i^2$ to neutral shell separation.

As relative velocity of shells decreases, charge exchange falls to zero.

initially ion shells accelerate

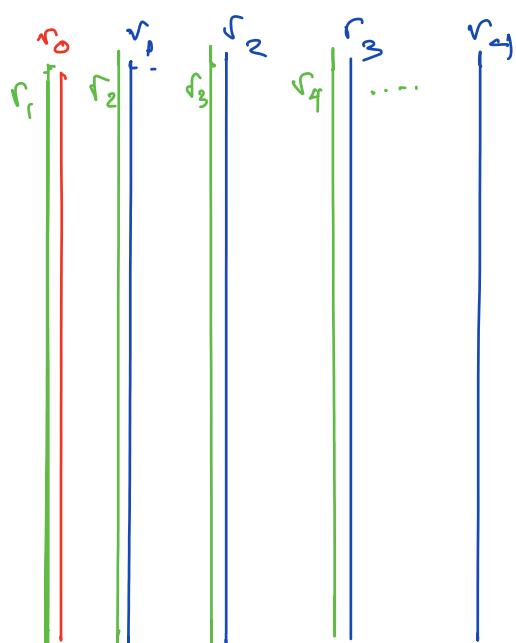
$$\ddot{u}_i = \frac{k_B T_e(t)}{m R(t)^2} r_i \quad \text{self-similar expand}$$





as ions expand, NO^+ ions react w/ Rydbergs
 $e^- + \text{NO}^+ + \text{Rydberg} \rightarrow 2\text{NO}^{**}$

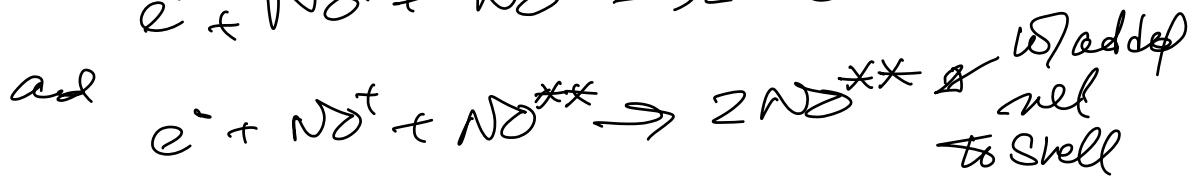
The two NO^{**} products populate shells moving w/ $\frac{1}{2}$ the ballistic velocity



Each wave of ions through the static NO^* shells sweeps up more Ryd density, transfers to the NO^{**} shells

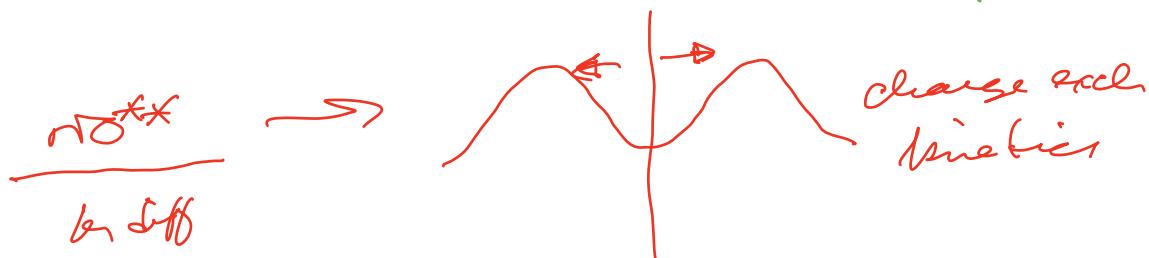
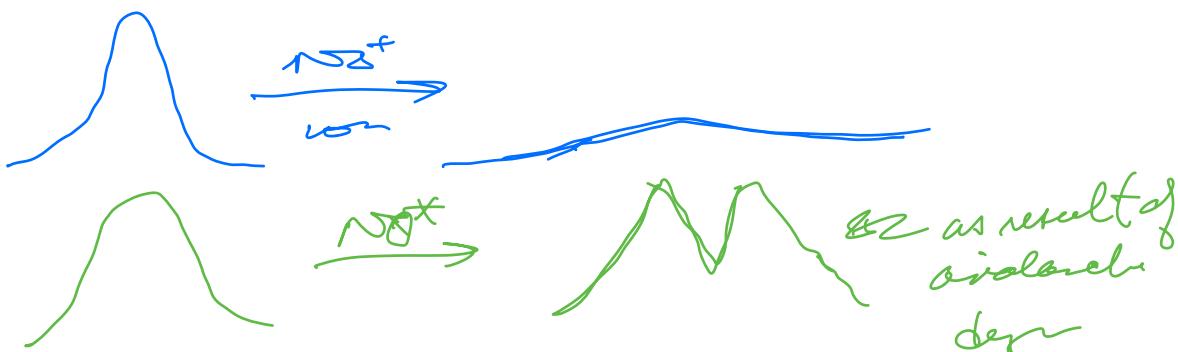
neglect reaction of $\text{NO}^+ + \text{NO}^{**}$
 (velocity matching reduces the rel vel
 \Rightarrow slow rate)

could correct for this by
partitioning the reaction
between



to first approx neglect the net $\frac{\text{W added}}$
treat ND^{**} the same as ND^*
continue to add $\frac{1}{2}$ the ion every
to the velocity of the moving
shell

at the end of expansion time,





To introduce asymmetry
in charge exchange, Run
two shell model calculations

Run 1 with Vlasov Gaussian
ellipsoid expansion plus
charge exchange tailored to
the yz plane (actually y axis)



1. Ion shells expand according to

$$r_i = \frac{k_B T_e(t)}{m_{N^+} \Gamma(t)^2} r_i$$

2. Calculate reactions within shells according to



$$\Delta [NO^{**}] = k_{NO^*}^{CT}(t) [NO^+] [NO^*] \Delta t$$

where Δt = time for NO^* shell boundary i to advance one unit and align with NO^* shell boundary $k+1$ (and so on)

the rate constant:

$$k_i^{CT} = \gamma_{CT} \cdot v_{NO^*}^i(t)$$

Where $v_{NO^*}^i(t)$ is the velocity with which the NO^+ shell boundary i passes through NO^* shell k . This quantity is simply $\frac{r_{k+1} - r_k}{\Delta t}$

We assume here that Δt is the same for every cell transit. That is every cell boundary i receives the same time Δt to advance from NO^* boundary k to $k+1$

3. Charge transfer adds population to a developing NO^{**} ellipsoid that advances with γ_2 of the instantaneous velocity of the NO^+ ellipsoid

At time $t=0$ the empty NO^{**} ellipsoid superimposes on the NO^+ ellipsoid.

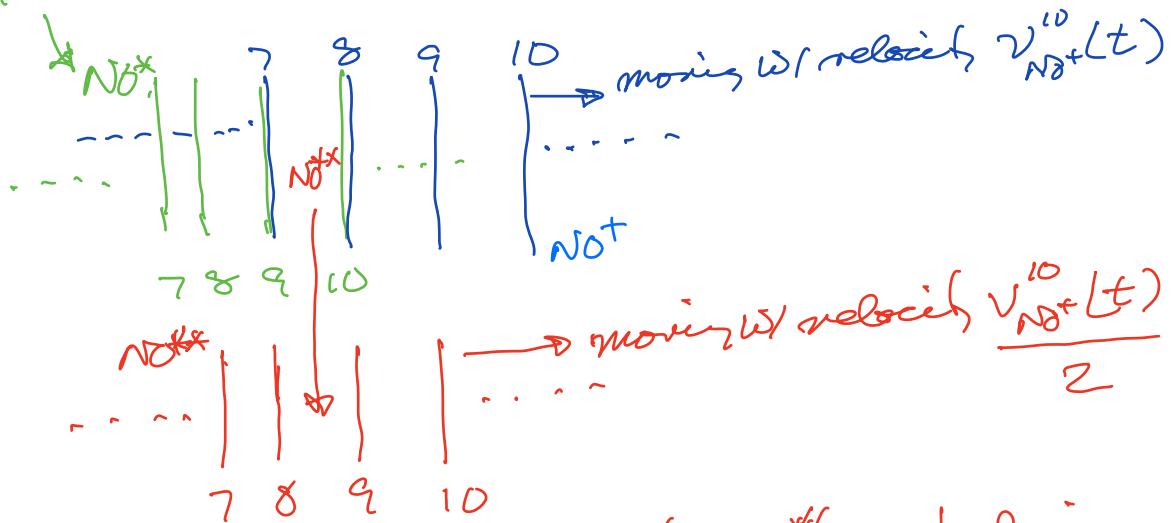
As time increases this ellipsoid advances according to

$$\dot{r}_i^{**} = \frac{1}{2} \frac{k_B T_e(t)}{m_{\text{NO}}^+ \Gamma(t)^2} r_i$$

Where r_i = radial distance of the NO^+ ion shell for $i = k$
 (the driving force for NO^{**} expansion remains solely NO^+ expansion)

4. We populate the NO^{**} shells by local charge transfer reaction.

stationary After some time t ,



charge transfer NO^{**} created in time t when NO^+ shell wall 8 moves from NO^+ shell wall 9 to NO^{**} shell wall 10 adds to NO^{**} shell between 8 and 9

5. As simulation proceeds

- NO^+ ellipsoid advances approx ballistically (because $T_e(t)$ falls) and loses NO^+ ions

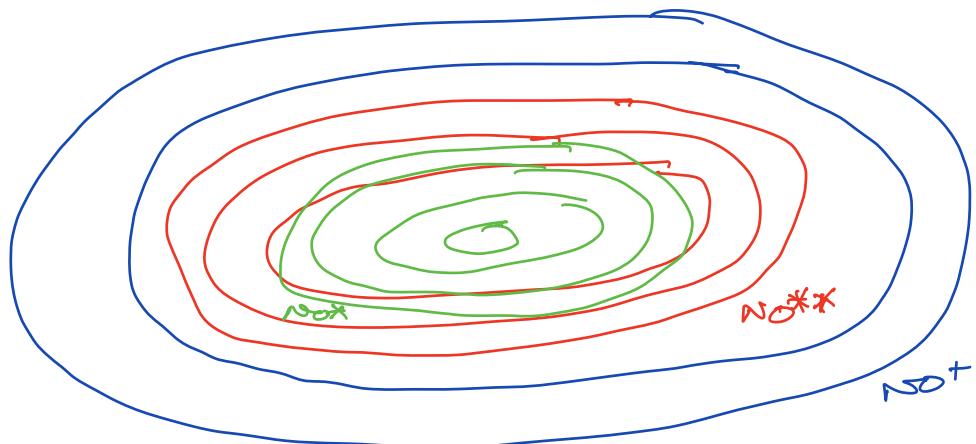
- NO^{**} ellipsoid advances ballistically

at $\frac{1}{2}$ the velocity for each shell wall (preserving the Gaussian self similar slope)

- NO^+ ions react with NO^* Rydberg molecules (fastest when populations overlap well) reducing $[\text{NO}^*]$ & $[\text{NO}^+]$ density in affected shells.
This reaction adds population locally to the nearest NO^{**} shells

In this simulation, if the -
reaction shell spacing
will proceed faster with lower
yield of NO^* .

At the end of simulation the
ellipsoid will appear as



NO^+ ellipsoid = Broad Gaussian with peak density still in the centre

NO^* ellipsoid unchanged shape but very low density (lost to predation and charge transfer)

NO^{**} ellipsoid donut with density only in shells that have happened to overlap with shells during intervals of Δt when CT occurs (other NO^* and NO^{**} populations both non-zero)

Save a movie of NO^+ density as a function of time and NO^{**} density as a function of time

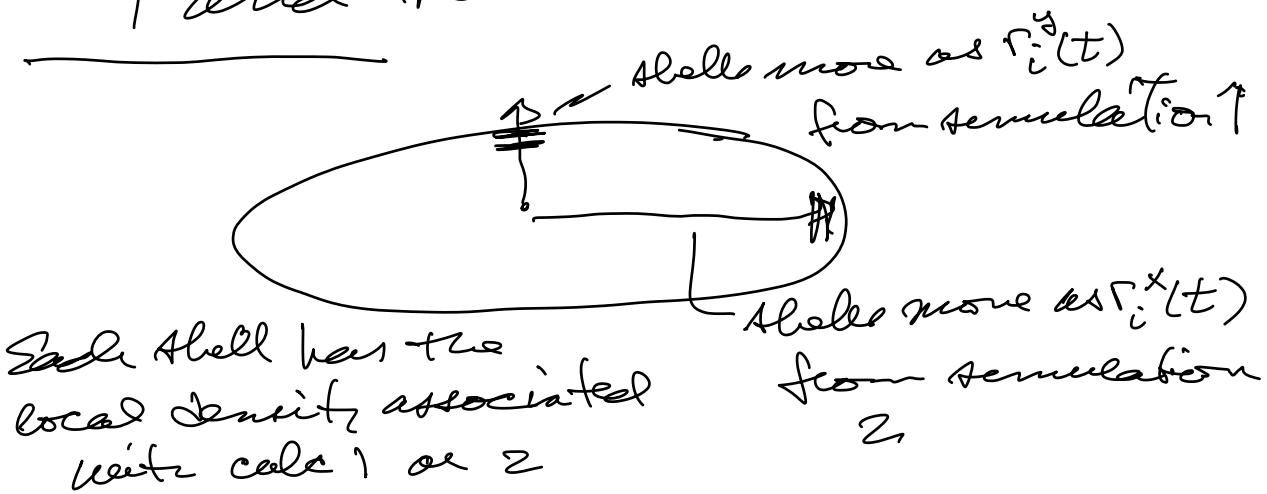
Question: how does standard model 3br and precipitation affect the scavenging density of NO^+ ? Assume NO^{**} totally labile

Run 2

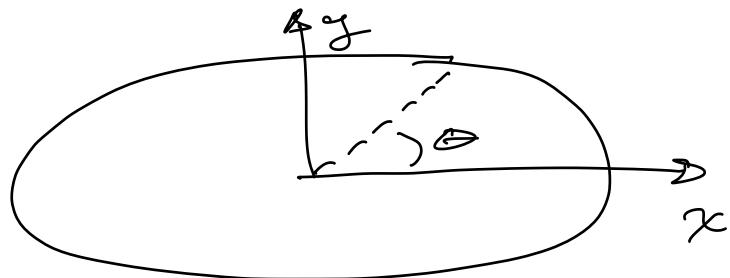
Perform the same simulation with Gaussian self-similar expansion rates (in $\text{m} \text{ s}^{-1}$) and shell boundaries figured with reference to X axis dimensions. Slower expansion and perhaps the larger shell widths, will increase local volumes of $\text{NO}^+ + \text{NO}^{**} \rightarrow 2\text{NO}^{**}$ conversion to NO^{**} filling the hollow NO^{**} ellipsoid

Run Simulation 1 and
 simulation 2 to completion
 for a given initial density
 and principal parameter number
 P_0 and n_0 .

Make a composite time-dependent
 ellipsoidal map that figures
 r_i^y and r_i^x shell dimensions
 along y and x as a function
 of time according to simulation
 1 and simulation 2



Having established the NB^{**}
 shell boundary dimensions
 and densities along y and x
 axes, compute the densities
 between as smooth functions
 of θ from $\pi/2$ to 0



Display this map of NB^{**}

It should look like

