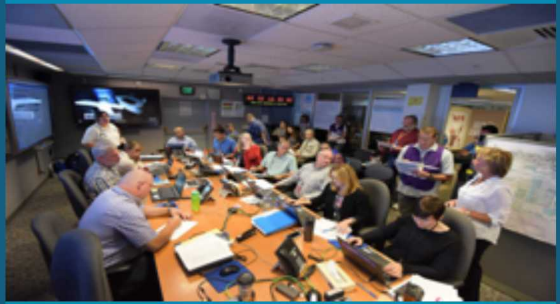
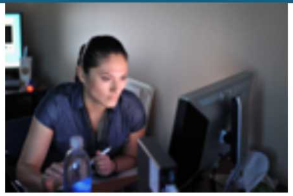
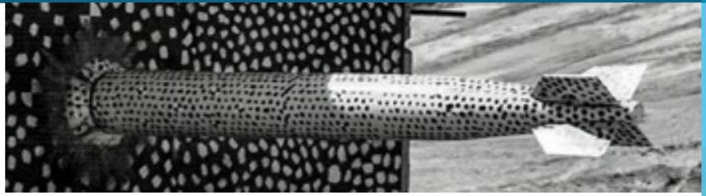
SAND2020-5705PE



ZA Model-to-Model Comparisons

05/07/2020





PRESENTED BY

Erin Mussoni

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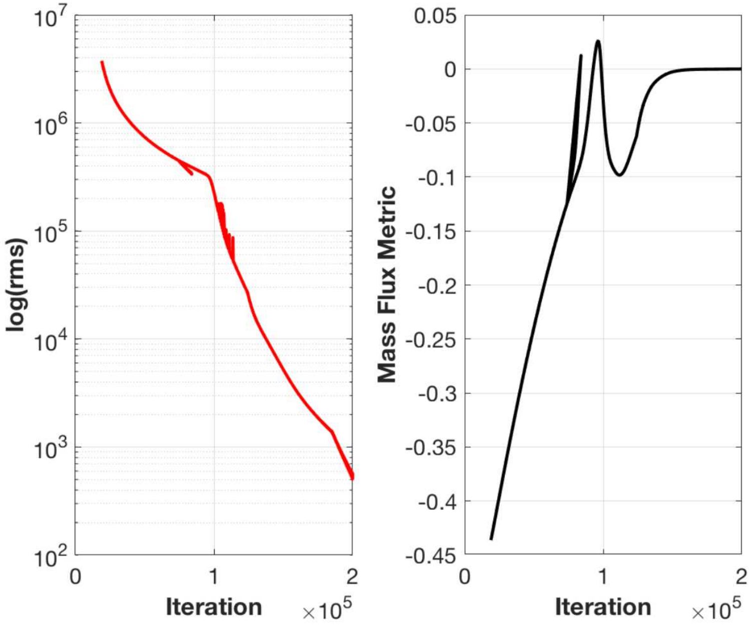
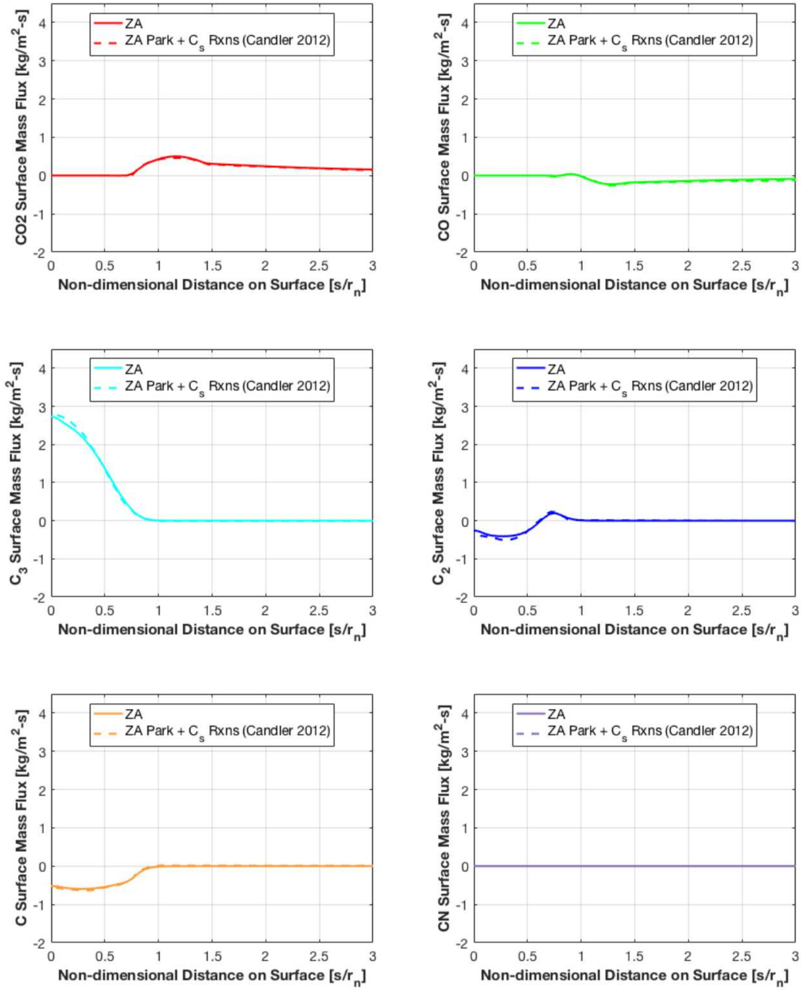
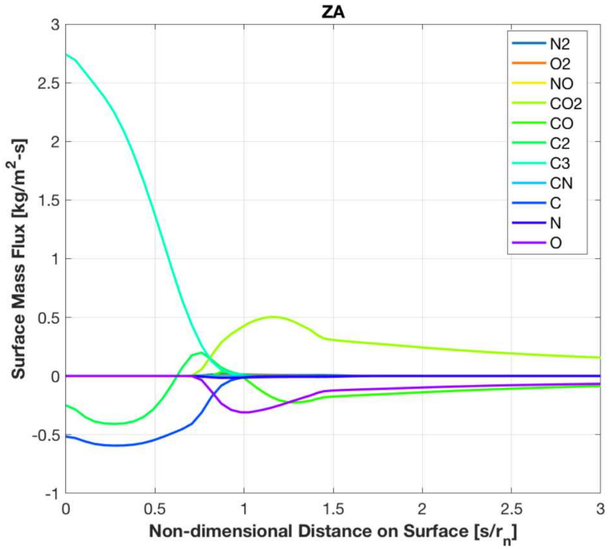
SAND2020-XXXX

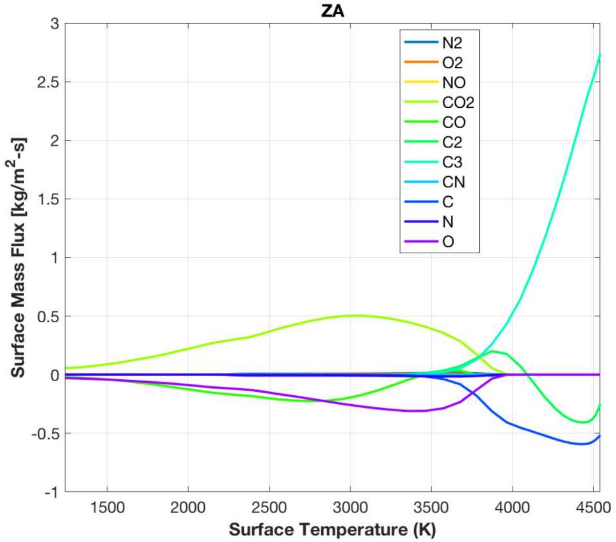
ZA Results for Altitude: 20 km



It's starting to begin the process of oscillating, which ends up growing around 10^2 – why is this? I was playing with the run schedule to see if I could delay it and get the rms lower.



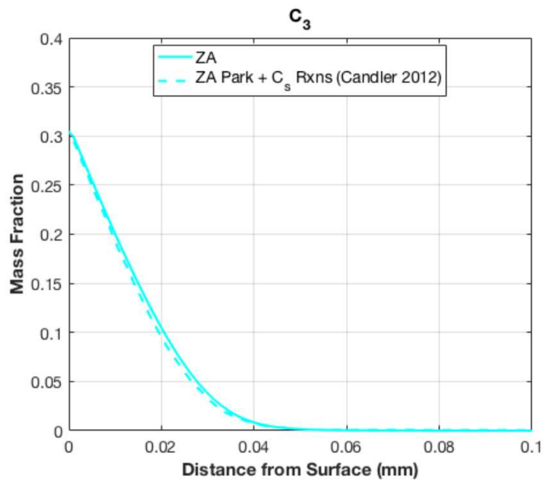


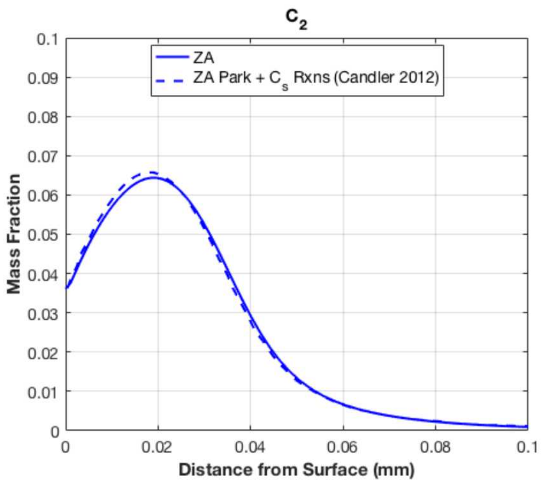


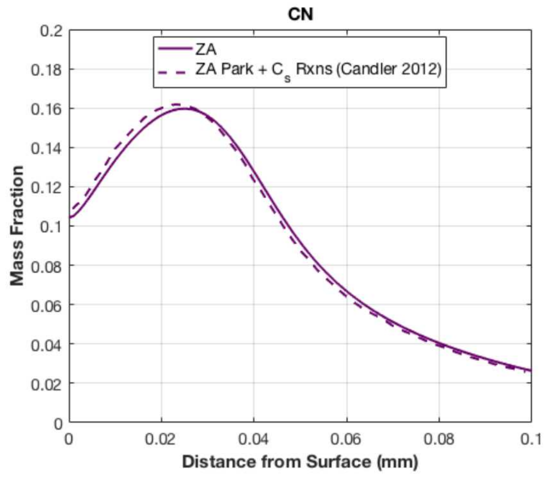
Species surface mass fluxes as a function of normalized distance from the stagnation point.

velocity: 7 km/s

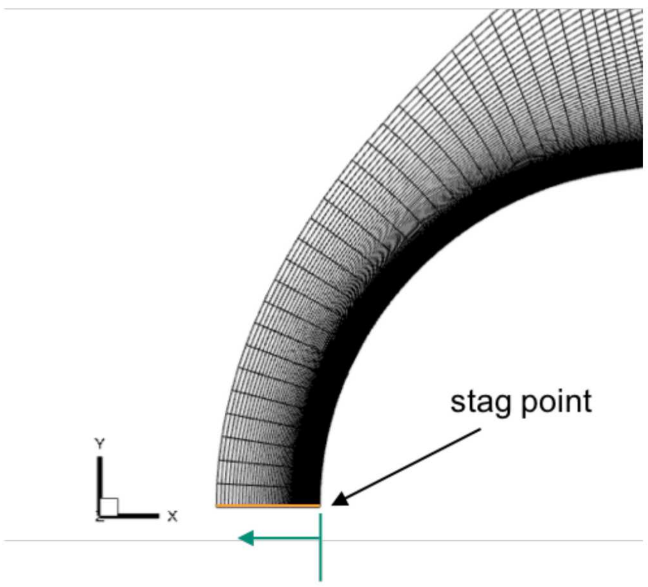
ZA Results for Altitude: 20 km





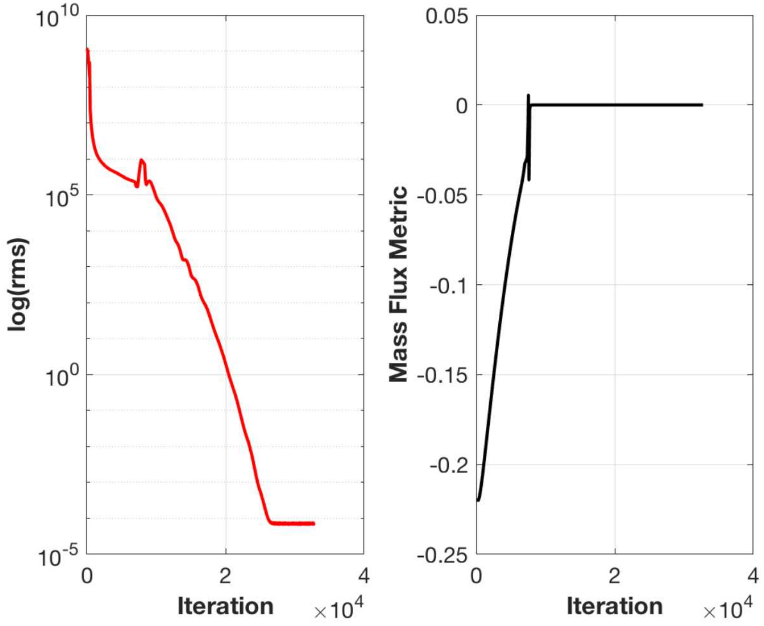


Where are we taking data?

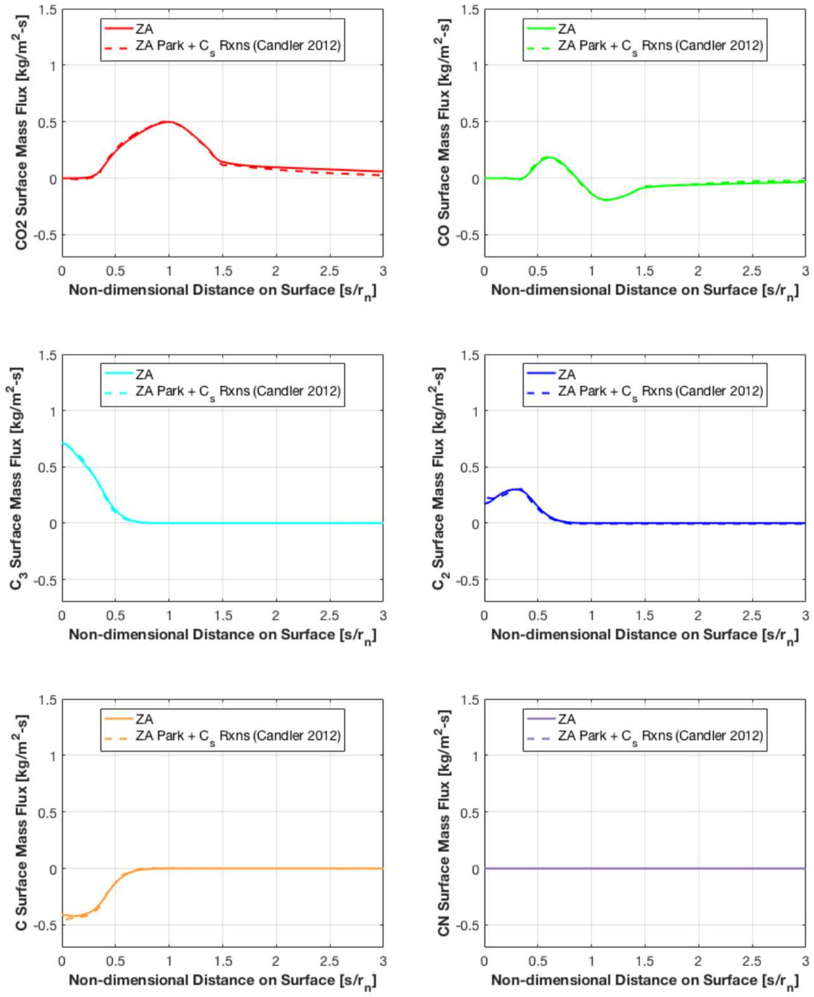


Species mass fraction as a function of surface-normal distance at the stagnation point.

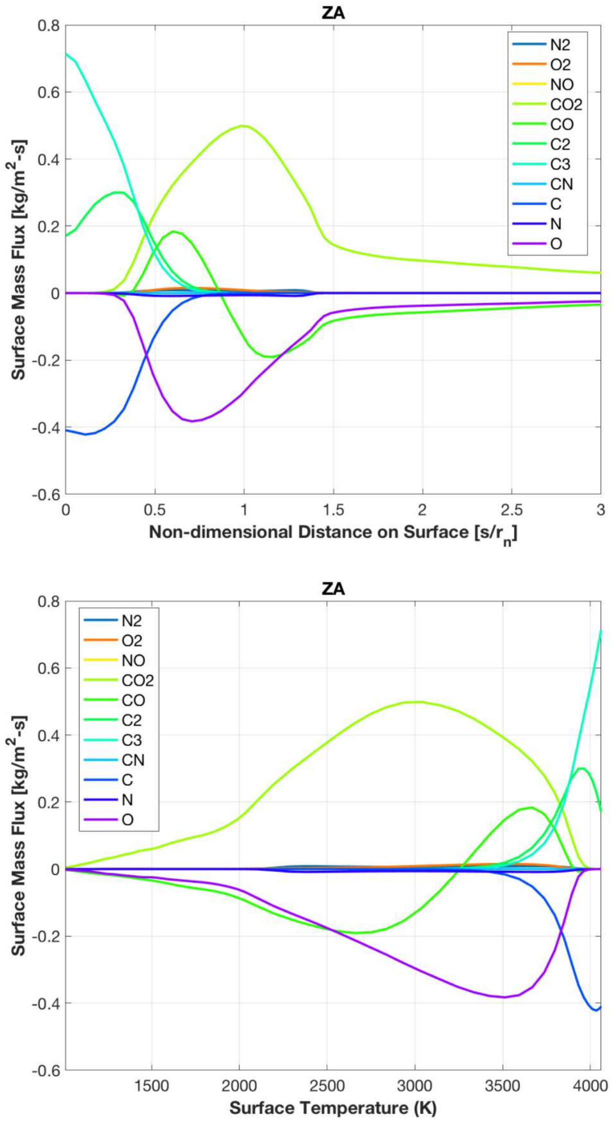
ZA Results for Altitude: 25 km



This was a process to get the CFL schedule working, but it was the easiest out of the two other cases. I babied it a lot until it spiked a little and ramped it up there. It seemed to settle after, so I didn't baby it any more.

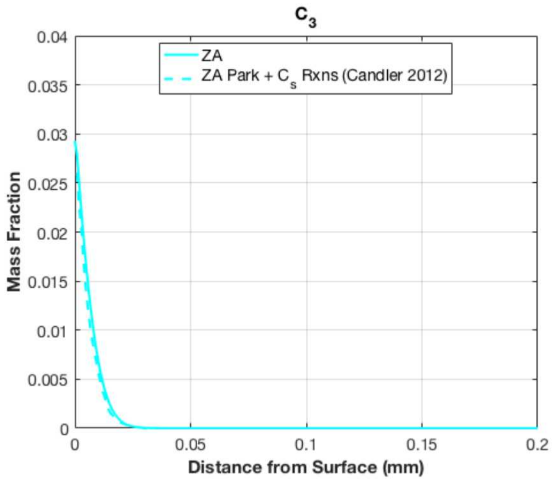


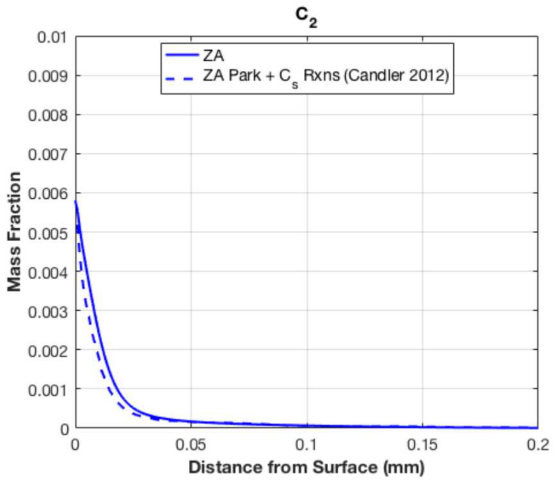
Species surface mass fluxes as a function of normalized distance from the stagnation point.

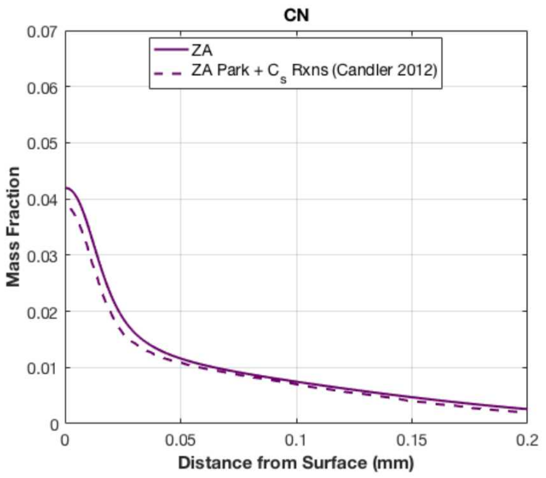


velocity: 7 km/s

ZA Results for Altitude: 25 km

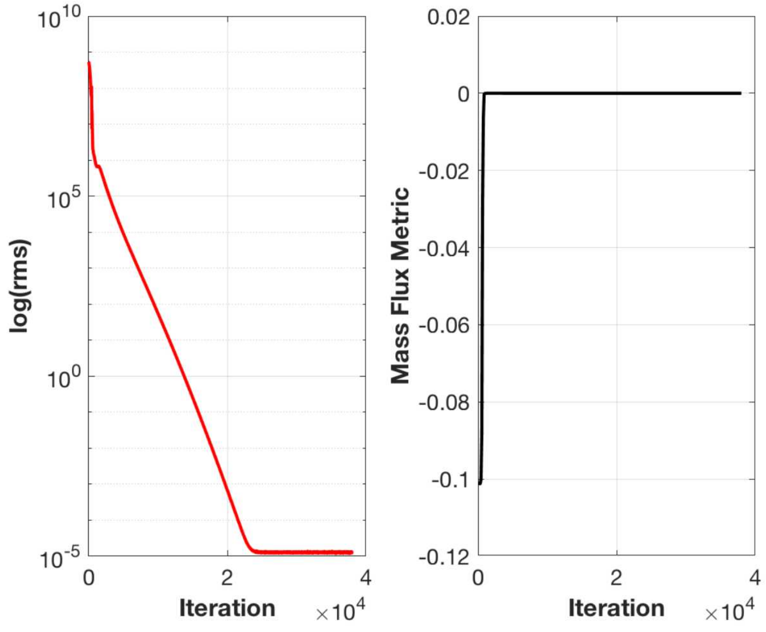




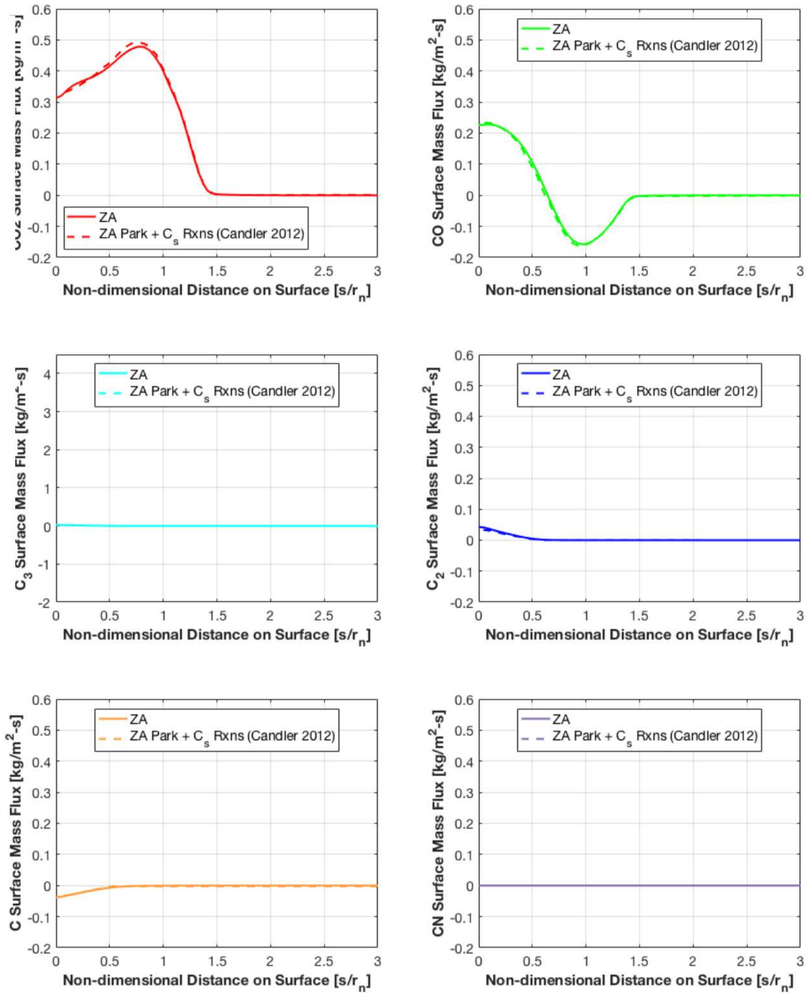


Species mass fraction as a function of surface-normal distance at the stagnation point.

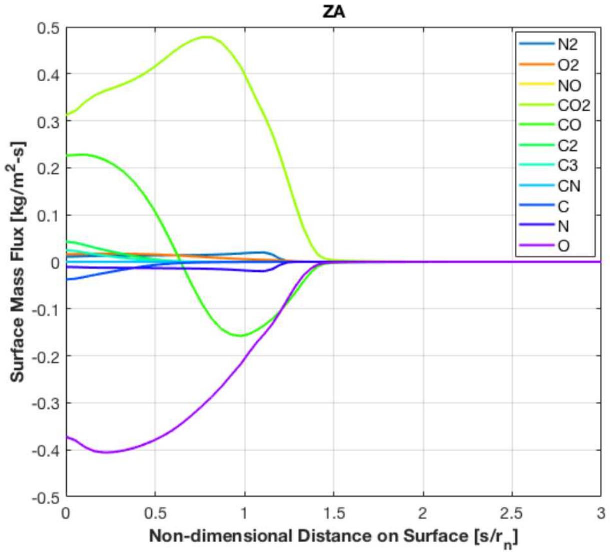
ZA Results for Altitude: 30 km

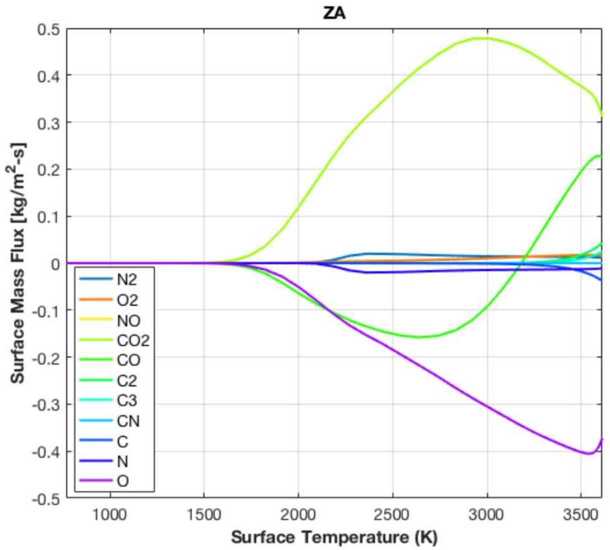


Started with schedule from zatest from Olivia's run



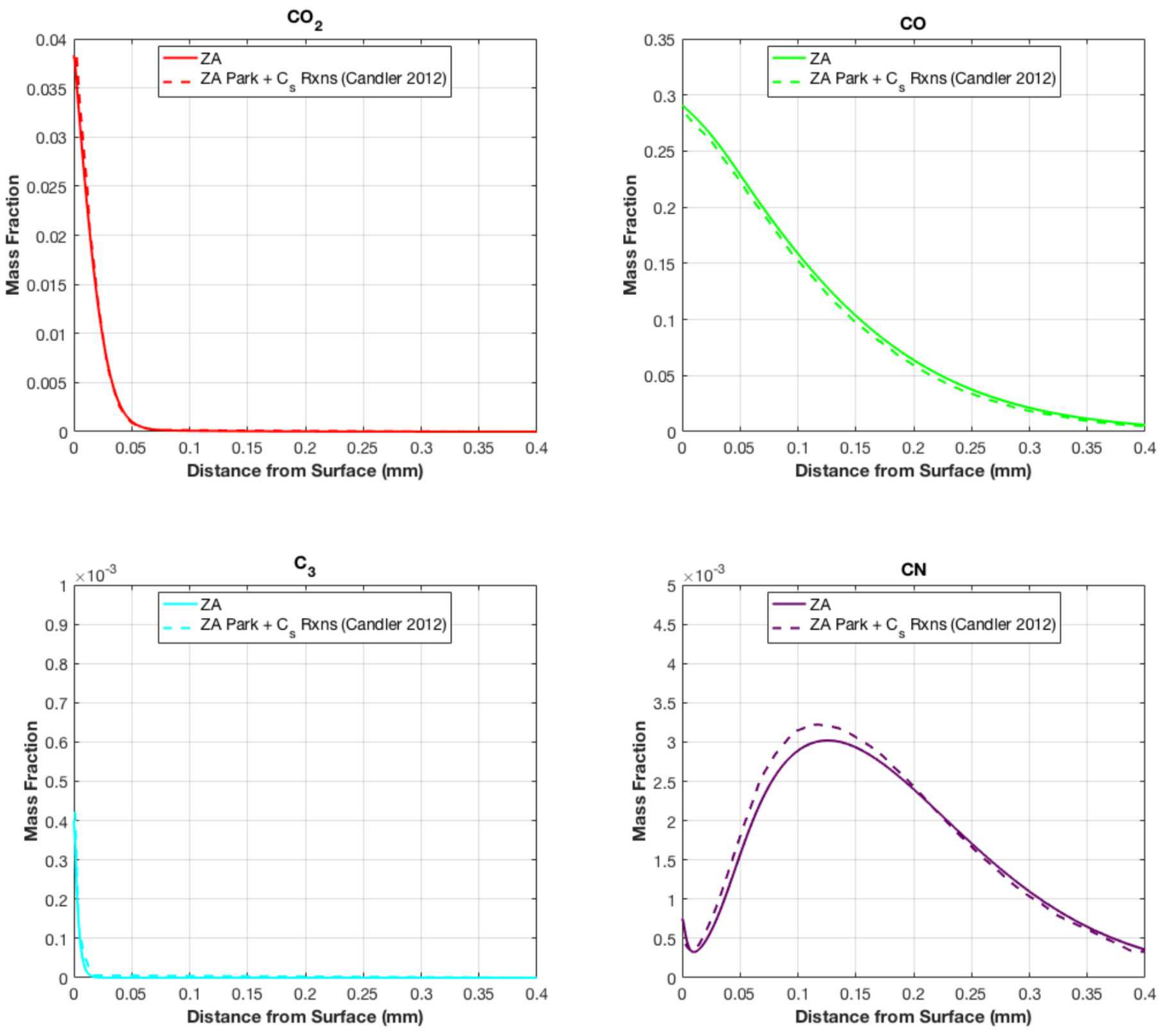
Species surface mass fluxes as a function of normalized distance from the stagnation point.





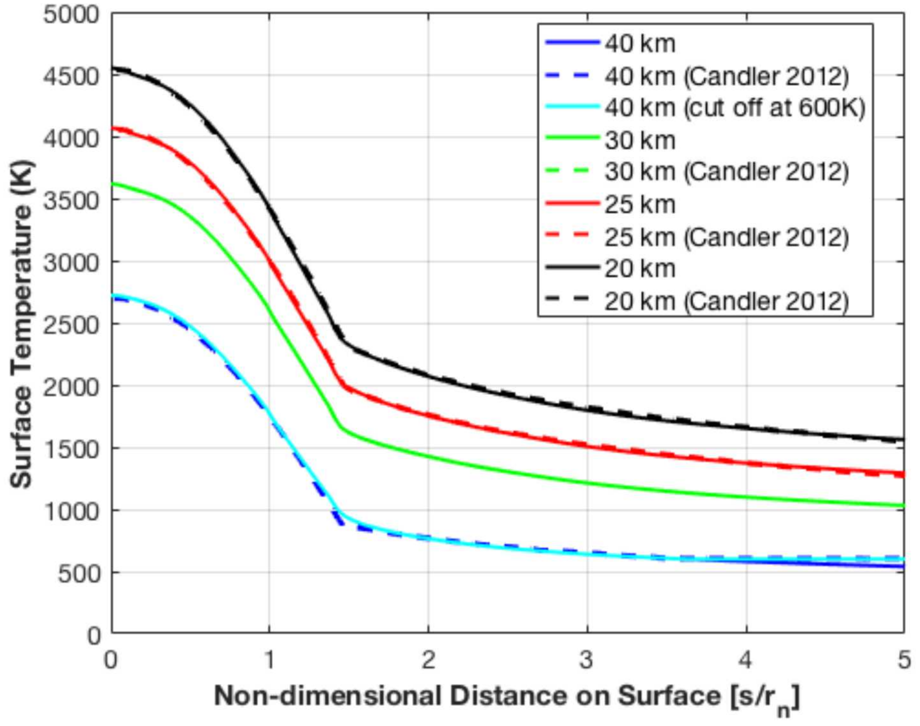
velocity: 7 km/s

ZA Results for Altitude: 30 km



Species mass fraction as a function of surface-normal distance at the stagnation point.

ZA Results for Altitude: 40 km



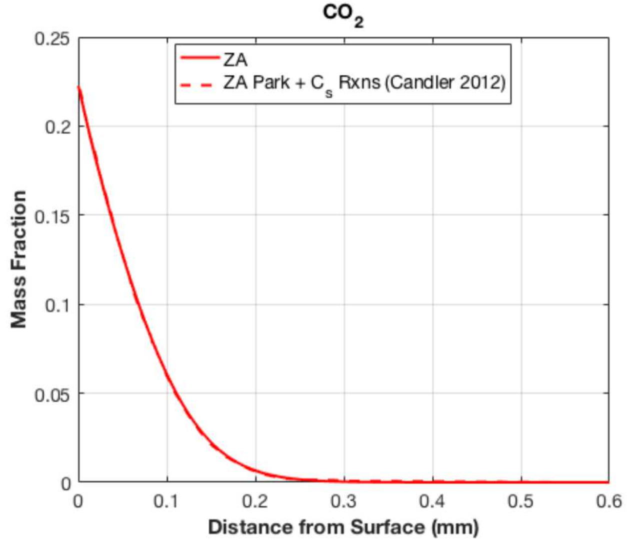
Updated Tsurf to cut off temperatures below 600 K (looks like Graham DID do this!)

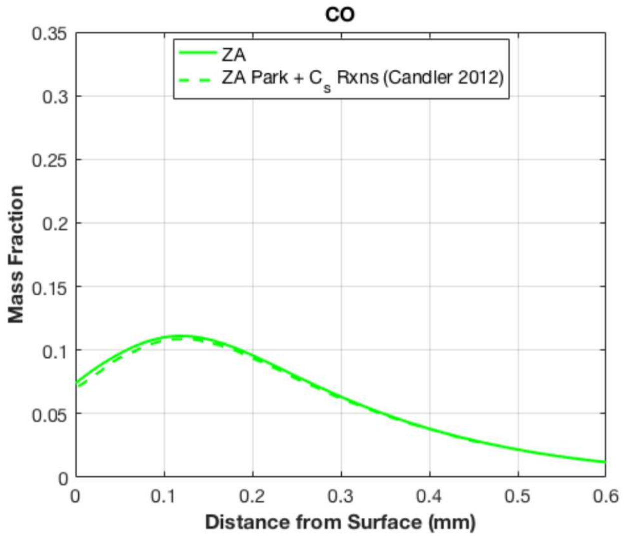
- Plotted new surface temperature profile in cyan
- This fixed my CFL run schedule woes. The run ended up being pretty robust and used the same run schedule as the 30 km case.

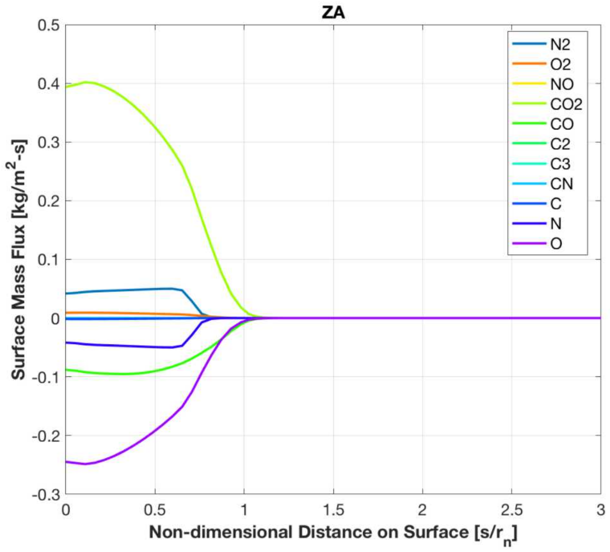
Will work on getting B' running better for all…

velocity: 7 km/s

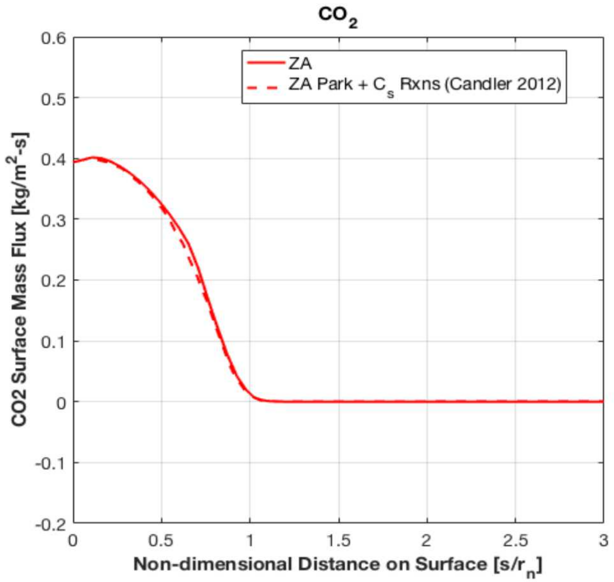
ZA Results for Altitude: 40 km

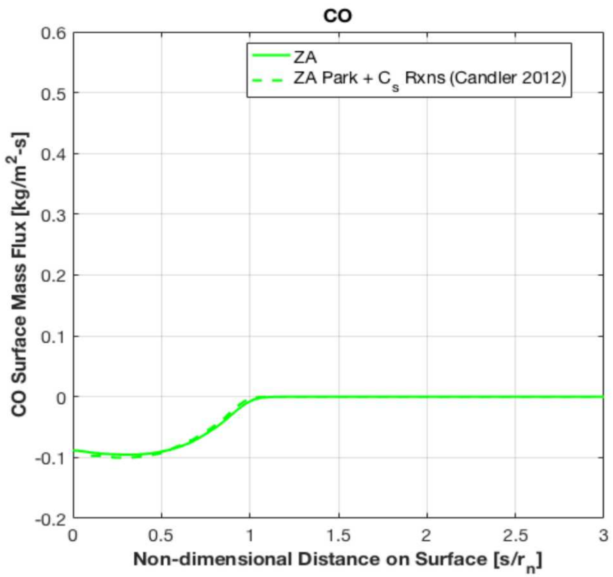


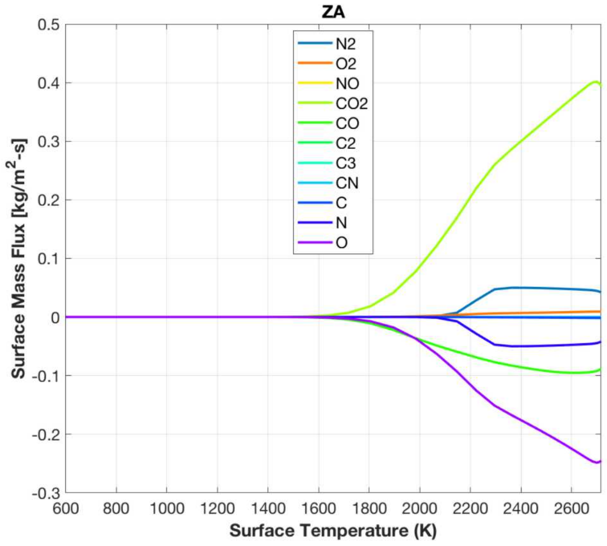




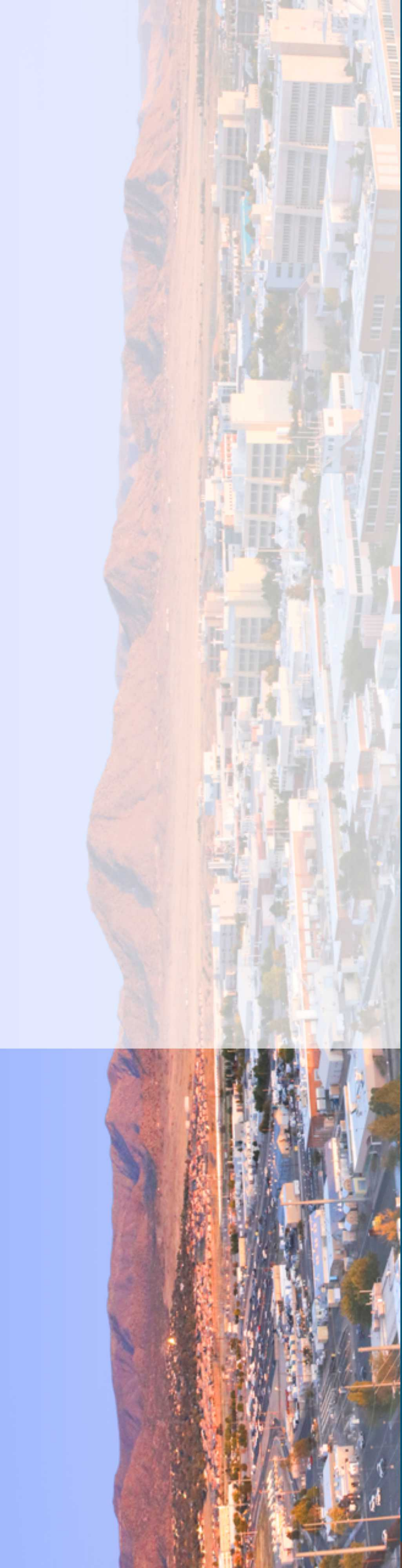
Species mass fraction as a function of surface-normal distance at the stagnation point.







Species surface mass fluxes as a function of normalized distance from the stagnation point.



Air Chemistry Model

What we are using:

```
[US3D_GAS_CHEMISTRY]
! ----------------------------------------------------------------------
format_version = 1
[/US3D_GAS_CHEMISTRY]

[GAS_SPECIES]
N2,O2,NO,CO2,CO,C2,C3,CN,C,N,O
[/GAS_SPECIES]

[GAS_REACTIONS]
! ----------------------------------------------------------------------
! Reaction list
!
! Type          Equation                          Cfm          eta          Ea           irxon    txf    txb
  diss    |     CO2 + M   <=> CO  + O  + M   |                 -1.50d+00, 6.3275d+04,  1,      0.5,   1.0
  diss    |     CO  + M   <=> C   + O  + M   |                 -1.00d+00, 1.2900d+05,  1,      0.5,   1.0
  diss    |     N2  + M   <=> N   + N  + M   |                 -1.60d+00, 1.1320d+05,  1,      0.5,   1.0
  diss    |     O2  + M   <=> O   + O  + M   |                 -1.50d+00, 5.9500d+04,  1,      0.5,   1.0
  diss    |     NO  + M   <=> N   + O  + M   |                  0.00d+00, 7.5500d+04,  1,      0.5,   1.0
  diss    |     C2  + M   <=> C   + C  + M   |                  0.00d+00, 6.9900d+04,  1,      0.5,   1.0
  diss    |     CN  + M   <=> C   + N  + M   |                  0.00d+00, 7.1000d+04,  1,      0.5,   1.0
  diss    |     C3  + M   <=> C2  + C  + M   |                  0.00d+00, 6.9900d+04,  1,      0.5,   1.0
  exch    |     NO  + O   <=> O2  + N        |    8.400d+09,  0.00d+00, 1.9400d+04,  1,      1.0,   1.0
  exch    |     N2  + O   <=> NO  + N        |    6.400d+14, -1.00d+00, 3.8400d+04,  1,      1.0,   1.0
  exch    |     CO  + O   <=> O2  + C        |    3.900d+10, -0.18d+00, 6.9200d+04,  1,      1.0,   1.0
  exch    |     CO  + C   <=> C2  + O        |    2.000d+14, -1.00d+00, 5.8000d+04,  1,      1.0,   1.0
  exch    |     CO  + N   <=> CN  + O        |    1.000d+11,  0.00d+00, 3.8600d+04,  1,      1.0,   1.0
  exch    |     N2  + C   <=> CN  + N        |    1.100d+11, -0.11d+00, 2.3200d+04,  1,      1.0,   1.0
  exch    |     CN  + O   <=> NO  + C        |    1.600d+10,  0.10d+00, 1.4600d+04,  1,      1.0,   1.0
  exch    |     CN  + C   <=> C2  + N        |    5.000d+10,  0.00d+00, 1.3000d+04,  1,      1.0,   1.0
  exch    |     CO2 + O   <=> O2  + CO       |    2.100d+10,  0.00d+00, 2.7800d+04,  1,      1.0,   1.0
  exch    |     C2  + C2  <=> C3  + C        |    3.000d+09,  0.00d+00, 0.0000d+00,  1,      1.0,   1.0
  exch    |     O   + C3  <=> CO  + C2       |    3.000d+10,  0.00d+00, 0.0000d+00,  1,      1.0,   1.0
  exch    |     N   + C3  <=> C2  + CN       |    3.000d+09,  0.00d+00, 0.0000d+00,  1,      1.0,   1.0
[/GAS_REACTIONS]

[GAS_REACTION_PARAMETERS]
! ----------------------------------------------------------------------
! Collision constants for each nrd reaction
!
   1~8:6.9000d+18     9~11:1.4000d+19
   1~8:2.3000d+17     9~11:3.4000d+17
   1~8:7.0000d+18     9~11:3.0000d+19
   1~8:2.0000d+18     9~11:1.0000d+19
```

From Candler 2012:

III.A. Gas-Phase Kinetics Models

To complete the carbon ablation model, we need an appropriate set of gas-phase reactions. Here, we will consider a gas composed of species: N_2, O_2, NO, CO_2, CO, C_2, C_3, CN, C, N, and O. There are several air-carbon kinetics mechanisms available in the literature; the most widely used model is due to Park et al.[5,6] A more recent compilation by Martin and Boyd[13] includes many additional reactions and chemical species related to phenolic decomposition. Here, we will start with the basic Park mechanism, and augment it with several additional reactions, including the reactions identified by Martin and Boyd as relevant under these conditions.

The basic Park kinetic mechanism for the 11-species model considered here is:

$$
\begin{array}{c|c}
CO_2 + M \leftrightarrow CO + O + M & NO + O \leftrightarrow O_2 + N \\
CO + M \leftrightarrow C + O + M & N_2 + O \leftrightarrow NO + N \\
N_2 + M \leftrightarrow N + N + M & CO + O \leftrightarrow O_2 + C \\
O_2 + M \leftrightarrow O + O + M & CO + C \leftrightarrow C_2 + O \\
NO + M \leftrightarrow N + O + M & CO + N \leftrightarrow CN + O \\
C_2 + M \leftrightarrow C + C + M & N_2 + C \leftrightarrow CN + N \\
CN + M \leftrightarrow C + N + M & CN + O \leftrightarrow NO + C \\
C_3 + M \leftrightarrow C_2 + C + M & CN + C \leftrightarrow C_2 + N \\
 & CO_2 + O \leftrightarrow O_2 + CO
\end{array}
$$

In particular, note that the only means for destroying C_3 is through the dissociation reaction $C_3 + M \leftrightarrow C_2 + C + M$. However, we would expect the possibility of direct oxidation and nitridation of C_3. Therefore, we have added three reactions:

$$
\begin{array}{c}
C_2 + C_2 \leftrightarrow C_3 + C \\
O + C_3 \leftrightarrow CO + C_2 \\
N + C_3 \leftrightarrow C_2 + CN
\end{array}
$$

with rates taken from the literature. We will see that these reactions are very important under strong sublimation conditions.