Martian Atmospheric Chemistry

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Background: Measurements of Martian Atmosphere

- Mars-3 took *in situ* spectra that quantified the abundance of H, CO, and O at 220 km
- Viking 1 and 2 Landers successfully delivered *in situ* measurements of the atmosphere and ion composition of Mars between 120 and 200 km
  - Mass spec measured abundances of major species: CO_2, N_2, Ar, CO, O_2, NO and minor species: H_2, He, etc.
- Hubble Space Telescope and FUSE quantified H and H_2 abundances
- MEX made spectral measurements of H and O at 200 km
- MAVEN measured basic structure of the upper atmosphere (major species He, N, O, CO, N2, NO, O2, Ar, and CO2) and ionosphere from the homopause to above the exobase

Chemical Composition of Martian Neutral Atmosphere

- The neutral atmosphere consists primarily of CO_2
- CO, O, N_2, H_2, H, Ar, He, H_2O are the next 8 most common neutrals
- Note: We assume neutrality – the production and loss of ions will balance out (more on this later)

Chemistry 101

- Ionization: When electrically neutral atoms or molecules are energized to release an electron
  - Photoionization: A photon hits an atom or molecule with energy greater than the ionization potential

$$hv + A \longrightarrow A^{+} + e^{-}$$

  - Ionization by collision: A free electron collides with a atom/molecule and results in a positive ion and another electron

$$e^{-} + A \longrightarrow e^{-} + A^{-} + e^{-}$$

Chemistry 101 – Reactions

- Neutral + ion reaction
  - reactants $\longrightarrow$ products
  - Reaction rate 'K': the speed at which a chemical reaction takes place (cm^3s^{-1})
  - e.g. $H^+ + H_2 \longrightarrow H_2^+ + H$; $k = 1 * 10^{-9}$
- Electron recombination reaction
  - $e^- + A^+ \longrightarrow B + [C]$
    - (A^+: positive ion; B, C: neutral)
  - Electron recombination rate: the speed at which the recombination reaction takes place (loss rate)

$$\text{ER Rate} = \text{ERCoeff}\left(\frac{300}{T_e}\right)^{TD}$$

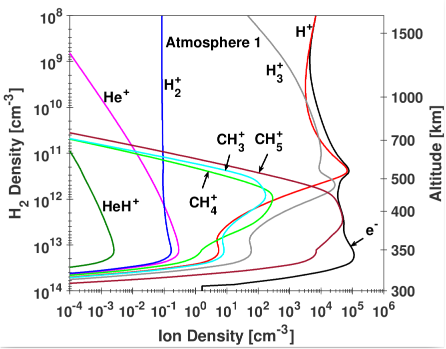
Where ERCoeff and TD are constants specific for the ion A^+ and T_e is electron temperature

Zero Sum Game

- A balance of recombination and electron loss is achieved in the Martian atmosphere (assumption)
  - No net charge
  - This restriction implies a "chemical network" of coupled equations
  - If there are 30 ion species, there are 30 equations and 30 unknowns $\implies$ solvable

Chemical Code

- General purpose: to produce a chemical model for Martian Atmosphere
  - Inputs: Neutral Density, Reactions List, Electron Temperatures, Secondary Production Rates
  - Outputs: Ion densities vs altitude for different ion species



Newton-Raphson Motivation

- Assumption: Production of ion J $=$ Loss of ion J (both functions of ion density)
- Let loss(J) – prod(J) $= f(x)$
- $\implies f(x) = 0 : x \in \mathbb{R}$
- Now we can solve for x (ion density)

Newton-Raphson Method

With an initial guess, x_0, we can solve $f(x) = 0$.
Then $x_1 = x_0 + \frac{f(x_0)}{f'(x_0)}$ where x_1 is the next best guess
and $x_2 = x_1 + \frac{f(x_1)}{f'(x_1)}$ where x_2 is the next best guess.

$$\implies x_{i+1} = x_i + \frac{f(x_i)}{f'(x_i)} \quad \text{for } i \in \mathbb{Z}^+$$

Note: The final result is independent of the initial guess. The number of iterations, however, can change as a result of changing initial guess (if maintaining the same goal accuracy).

Linear Algebra: Motivation

- What is $\frac{f(x_i)}{f'(x_i)}$?
  - The function multiplied by the multiplicative inverse of the derivative of the function.
  - Since we are dealing with coupled equations, we can represent this in matrix form.

Linear Algebra: Application

- Goal: Write $\frac{f(x_i)}{f'(x_i)}$ in matrix form
- Let n be the number of ions we are considering
- Let β(i) = Loss of ion 'i' − Production of ion 'i'
  - Loss of ion 'i' is from recombination
  - Production of ion 'i' is from ionization
  - Then $\beta \in \mathbf{M}_{nx1}$
- Let $\alpha \in \mathbf{M}_{nxn}$: such that α is the matrix of derivatives of the function with respect to the constituent roots
- Then $\frac{f(x)}{f'(x)} \longrightarrow \frac{\beta}{\alpha} = \alpha^{-1}\beta$

Linear Algebra: Inverse of α

- Goal: $\frac{f(x)}{f'(x)} \longrightarrow \alpha^{-1}\beta$
  - α is known, α^{-1} must be calculated
- Let I be the *nxn* multiplicative identity matrix. Then $\exists\ \gamma = [\alpha : \mathrm{I}]$ such that RRE$(\gamma) = [\mathrm{I} : \alpha^{-1}]$

Converting the rest of the scalar equation

- Goal: $x_{i+1} = x_i + \frac{f(x_i)}{f'(x_i)} \longrightarrow$ Vector Form
- Known: $\frac{f(x)}{f'(x)} \longrightarrow \alpha^{-1}\beta$
- What are x_{i+1} and x_i?
  - In the scalar form, they are guesses of a single species' ion density
  - Thus, in matrix form, $x_p \in \mathbf{M}_{nx1}$ where $p \in \mathbb{Z}$

$$x_{i+1} = x_i + \frac{f(x_i)}{f'(x_i)} \longrightarrow \boldsymbol{x}_{i+1} = \boldsymbol{x}_i + \alpha^{-1}\beta$$

- $x_{i+1} = x_i + \alpha^{-1}\beta$ is iterated until a certain accuracy is reached. The resulting x vector is then the approximation of the ion densities of n species.

References

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