Multifluid modelling of cometary coma for diverse range of parent volatile compositions

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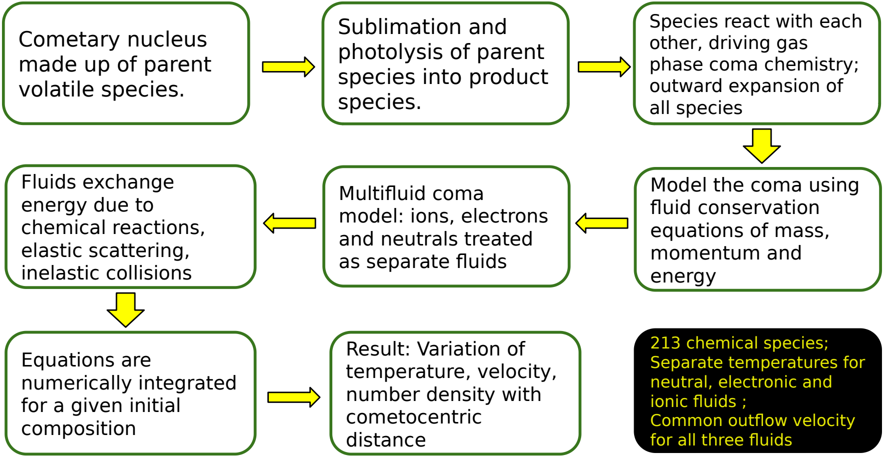
Introduction

- The volatile composition of the coma is generally diverse,
  - H_2O is mostly a primary constituent
  - followed by CO and CO_2
  - trace amounts of other species such as CH_4, CH_3OH, NH_3
- In some comets, the observed CO/H_2O ratios are $>> 1$.
- We model the coma with an aim to study how the chemistry and dynamics of the coma will change when we alter the relative abundances of the parent volatiles.

Coma model



Cometary nucleus made up of parent volatile species.

Sublimation and photolysis of parent species into product species.

Species react with each other, driving gas phase coma chemistry; outward expansion of all species

Model the coma using fluid conservation equations of mass, momentum and energy

Multifluid coma model: ions, electrons and neutrals treated as separate fluids

Fluids exchange energy due to chemical reactions, elastic scattering, inelastic collisions

Equations are numerically integrated for a given initial composition

Result: Variation of temperature, velocity, number density with cometocentric distance

213 chemical species;
Separate temperatures for neutral, electronic and ionic fluids ;
Common outflow velocity for all three fluids

Governing Equations: Conservation of number density, mass, momentum, energy

$$\frac{1}{r^2}\frac{d}{dr}(r^2 n v) = N \tag{1}$$

$$\frac{1}{r^2}\frac{d}{dr}(r^2 \rho v) = M \tag{2}$$

$$\frac{1}{r^2}\frac{d}{dr}(r^2 \rho v^2) + \frac{d}{dr}(n k_B T) = F \tag{3}$$

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2 \rho v\left(\frac{v^2}{2} + \frac{\gamma}{\gamma - 1}\frac{k_B T}{\mu}\right)\right] = Q \tag{4}$$

r: cometocentric distance, n: species number density, ρ: mass density, v: velocity, T: temperature, γ: ratio of specific heat

N, M, F, Q: source terms

Initial Conditions

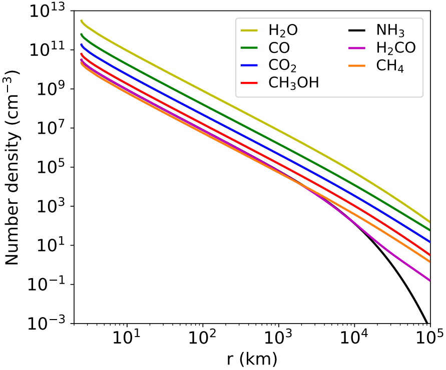
- Two cases studied; case A: H_2O is dominant, case B: CO is dominant
- Sublimation rate from the nucleus is 10^{29} molecules s^{-1}

Table: Species abundances as a percentage of the dominant parent volatile

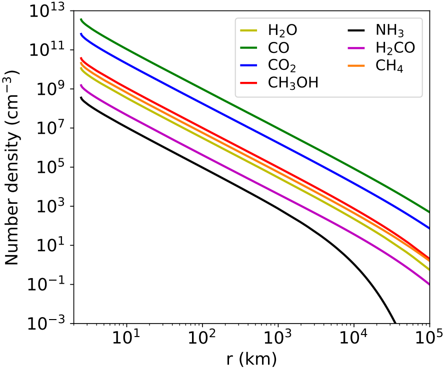
Parent Species	Case A[1] (Hyakutake)	Case B[2] (C/2016 R2)
H_2O	Dominant	0.32
CO	20.0	Dominant
CO_2	6.0	18.2
NH_3	1.0	0.010
HCN	0.1	3.8×10^{-3}
N_2	0.04	5.0
CH_4	0.7	0.59
CH_3OH	2.0	1.04
H_2CO	1.0	0.043
C_2H_2	0.1	0.022
C_2H_6	0.4	0.089

[1] S. D. Rodgers and S. B. Charnley, 2002, MNRAS, 330, 660 – 674 [2] Adam J. McKay *et al.*, 2019, AJ, 158, 128 (24pp)

Number density profile of parent volatiles



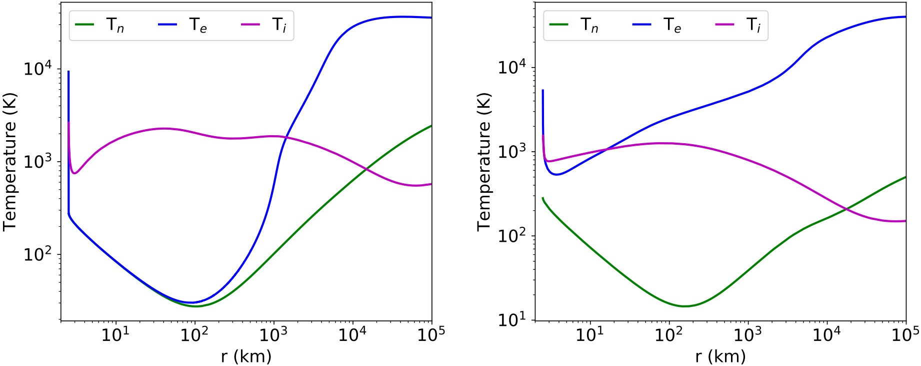
Case A



Case B

- The dominant parent volatile has the highest number density (H_2O in case A and CO in case B).
- Number density for most parent volatiles falls of roughly as $1/r^2$.
- Number density of NH_3 falls off faster in the outer regions due to higher photodissociation.

Temperature profile

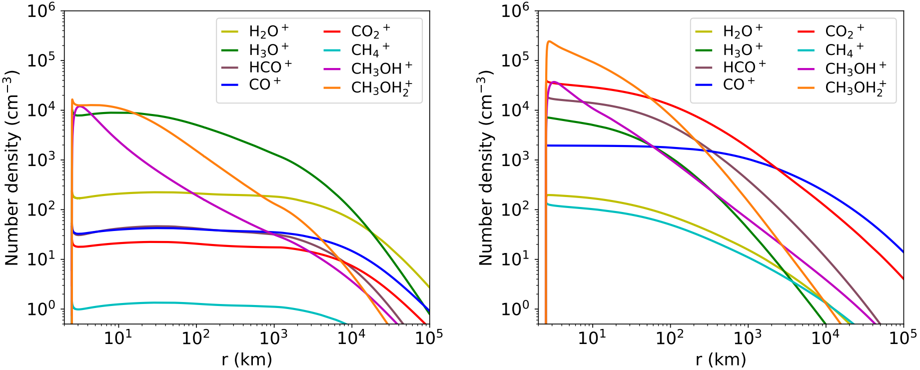


Case A

Case B

- Subscripts *n*, *e* and *i* denote neutral, electron and ion fluids respectively.
- Initial temperature coupling between *n* and *e* fluids in case A; large electron-H_2O inelastic collision cross-section and high density results in efficient energy exchange. In outer region, coupling is lost due to reduced density.
- No such coupling in case B; electron-CO inelastic collision cross-section is nearly 3 orders of magnitude less than that of electron-H_2O.

Ionic density profile

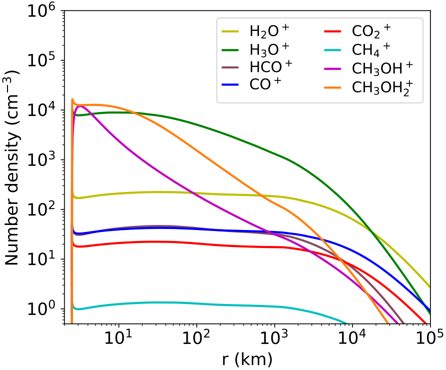


Case A

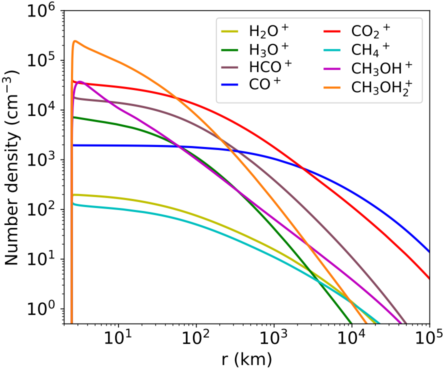
Case B

- Higher CO abundance in case B directly or indirectly results in higher abundance of the ions CO^+, CO_2^+ and HCO^+ by nearly $2-3$ orders.
  - CO^+ primarily produced by photoionization of CO.
  - CO_2^+ mainly produced by charge exchange of CO_2 with CO^+.
  - HCO^+ produced when CO reacts with ionic species.

Ionic density profile



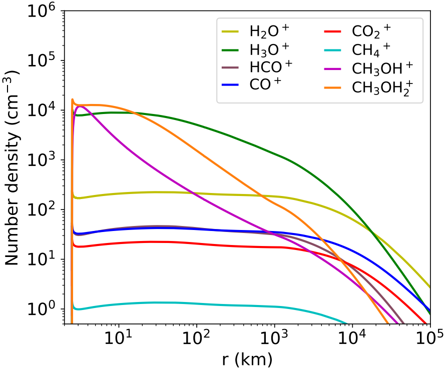
Case A



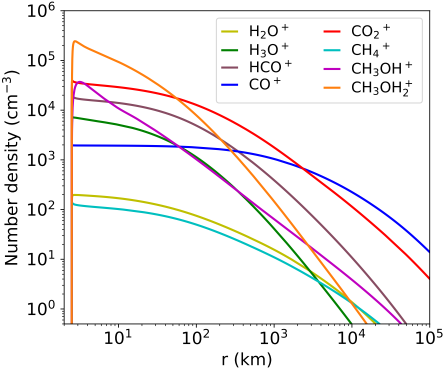
Case B

- Water derived ions H_2O^+ and H_3O^+ show similar abundance in the innermost regions in both cases, even though H_2O is much less in case B.
- The ions CO_2^+ and HCO^+ have higher abundance in case B, and these react with H_2O to produce H_2O^+ and H_3O^+ respectively.

Ionic density profile



Case A



Case B

- Bigger ions are more abundant in case B.
- CH_4^+ is created by photoionization of CH_4, and also by charge exchange of CH_4 with CO^+ and CO_2^+.
- CH_4^+ reacts with CH_3OH to form CH_3OH^+ and $CH_3OH_2^+$.

Conclusion

- The dominant parent species drives the physical and chemical conditions of the coma.
- The temperature profile differs in the two cases, due to different rates of exchange of energy betweeen the fluids.
- Ionic composition of the coma is affected by changes in the relative abundances of the parent volatiles.