NUMERICAL SIMULATION OF CHEMICAL REACTIONS WITHIN A VAPOR PLUME INDUCED BY COMETARY IMPACT.
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Introduction: Impacts have played an important role in the evolution of surface environment of planets, asteroids, and satellites. When the impact velocity is higher than about ten km/s, materials around the impact site and most of the impactor evaporate forming a vapor plume [1]. Since the temperature and pressure in the vapor plume are extremely high, the plume expands and cools rapidly. Chemical equilibrium within the vapor plume is achieved when the temperature and pressure of the vapor plume remain high. As the vapor plume expands and cools, the rate of chemical reaction decreases and eventually all the chemical reaction cease. As a result, various thermal disequilibrium compositions are left as end products [2]. Especially, in the case of cometary impact, a significant amount of hydrocarbons form since comets contain a large amount of C, H, O, and N.

Although the mechanical aspects of a cometary impact has been well studied [3-5], the chemical aspects of a cometary impact is not extensively studied because of (i) the limitation of the size in experimental study and (ii) the limitation of computational capability. Fegley et al. [6] estimated the HCN and CH_2O production by shock heating of atmosphere by bolide impact assuming (i) the chemical reactions cease instantly when the expansion rate of heated gas parcel defeats chemical reaction rate and (ii) the final abundance of each species is calculated as equilibrium abundance at the pressure-temperature condition at the moment of chemical reaction cessation. This simple model works well only when an equilibrium concentration changes very weakly as a function of a temperature near a quench temperature [7]. This model, however, may not be applied to chemistry within a vapor plume because equilibrium concentrations of some chemical species contained in the gas-phase chemistry within the vapor plume depends strongly on the pressure-temperature profile of a impact vapor plume.

Thus, in this study, we develop a new numerical code to simulate a gas-phase reaction network within an impact vapor plume formed by a cometary impact. We conduct numerical simulations for various impact conditions (e. g., a radius of comet and an impact velocity) that determine an initial condition of a vapor plume.

Numerical procedures: To simulate the gas-phase reaction network within the vapor plume, we incorporate a kinetics model (GRI Mech version 3.0) into hydrodynamic model [8] of the vapor plume. We develop a kinetics code by using the kinetic data for 325 elementary reactions and thermodynamics data for 53 compounds in a C/H/O/N systems taken from GRI Mech version 3.0 (http://www.me.berkeley.edu/gri_mech/). GRI Mech is a compilation of elementary reactions common to the combustion chemistry and is adequate for simulating a high-temperature and high-pressure chemistry within the vapor plume. To simulate the expansion of the vapor plume, we adopt a model of hydrodynamics [8] that can simulate a shock wave induced by an expanding vapor plume.

We assume that (i) a comet impacts onto an icy body without an atmosphere for simplicity, (ii) the vapor plume follows a radially symmetric (one-dimensional) motion and maintains a spherical shape and (iii) the vapor plume cools rapidly by adiabatic expansion. The equation of state of ideal gas is used. For coupling the kinetics model and the dynamics model, the hydrodynamic calculation feeds back reaction heat, mean molecular mass and specific heat ratio of a mixture gas derived from the kinetics calculation. We divide the vapor plume into 10 computational cells in which the kinetics calculation is conducted.

Here we use a monatomic gas mixture with a typical comet's composition (H : C : O : N = 30 : 8.1 : 1.4 : 18.8 [9]) as an initial compositions of the vapor plume. We estimate an initial pressure of the vapor plume from the Rankine-Hugoniot equation by assuming that both a projectile and a target is composed of a water ice. An initial specific energy E_0 of the vapor plume is taken to be $E_0 = (E - H)$ where E is a specific internal energy of the projectile that can be estimated from the planar

impact approximation [10]. H is the enthalpy of vaporization of the projectile (water ice).

We use eight different radii of comets (1 mm, 10 mm, 100 mm, 1 m, 10 m, 100 m, 1 km, and 10 km (K/T size)) and use four different impact velocities (7.5 km/s, 10 km/s, 12.5 km/s, and 15 km/s).

Results: An abundance of each species within the vapor plume finally reaches a constant value individually with cooling of the plume. We take the terminal constant abundance as the abundance of quenched end product within a vapor plume.

Fig. 1 shows molar fractions of end products as a function of the radius of comet at impact velocity of 10 km/s. It is clear that cometary size affects the abundances of chemical species; a smaller comet produces more NH_3, HCN, HNCO, CH_2O, C_2H_4, C_2H_2, C_2H_6 , and CH_3OH.

Fig. 2 shows molar fractions of end products as a function of impact velocity for radius of comet 100 m. It is clear that the impact velocity greatly affects the abundances of chemical species; a lower impact velocity produces more CH_4, NH_3, HCN, HNCO, CH_2O, C_2H_4, C_2H_6, and CH_3OH.

Discussion: Here, we discuss the effects of impact conditions such as the size and the impact velocity of comet.

Effects of comet size. Smaller radius of comet leads to shorter cooling time. Then, the chemical reaction quenches at a higher temperature. This accounts for our result that the smaller comet produces more NH_3, HCN, HNCO, CH_2O, C_2H_4, C_2H_2, C_2H_6, CH_3OH that are stable at a high temperature or at a high pressure.

Effects of impact velocity. The impact velocity controls the pressure-temperature profile of the vapor plume. The pressure-temperature profile of the vapor plume affects the abundance of the species. Then, the impact velocity may affect abundances of end products. Generally, the vapor plume formed under the impact condition of a low impact velocity cools maintaining high pressure. We can explain that the lower impact velocity produces more CH_4, NH_3, HCN, HNCO, CH_2O, C_2H_4, C_2H_6 and CH_3OH that are stable at a high pressure.

Our results suggests that the impact conditions greatly affect the amounts of hydrocarbons (CH_4, C_2H_2, C_2H_4, and C_2H_6), precursors of biomolecule (HCN and CH_2O) NH_3, and CH_3OH produced by gas-phase reactions within the vapor plume induced by the cometary impact. This implies that we need a framework of a planetary evolution including impact processes in which effects of impact conditions (a size and an impact velocity of a projectile) are taken into accounts.

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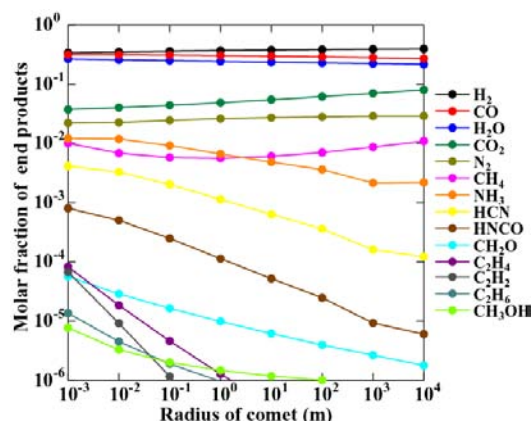

Fig. 1. Molar fractions of end products as a function of a radius of comet. Impact velocity is 10 km/s.
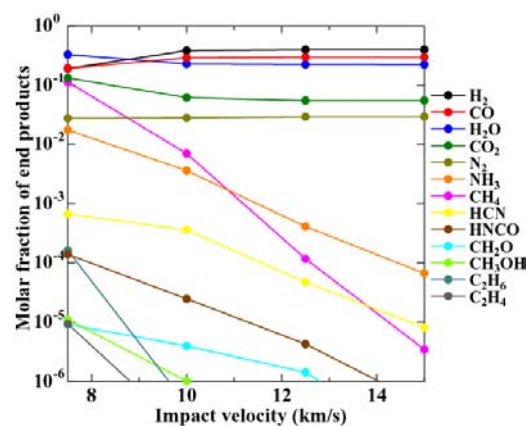

Fig. 2. Molar fractions of end products as a function of a impact velocity. Radius of comet is 100 m.