Wind Tunnel and CFD Studies on Production of Prebiotic Materials in Hypersonic Flow around Extraterrestrial Entry Object

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Abstract

To investigate the possibility of prebiotic materials formation in high temperature shock layer around an ablating icy object entering the early earth's CO_2/N_2 atmosphere, the cooperative research of the CFD and EFD has been conducted. The thermo-chemical nonequilibrium Navier-Stokes analysis shows that HCN is efficiently produced in the stagnation region and transported into the atmosphere by the wake flow. To simulate such process experimentally in the hypersonic air flow of the wind tunnel, the experimental model composed of the ablative nose part made from water ice and dry ice to supply the C and H elements and the after-body having the electric discharge circuit in it to supply the energy necessary for chemical reactions has been designed, based on the CFD results. We observed the emission from CN in the wind tunnel, and better understanding about the phenomena is expected by comparison with the CFD analysis.

Key words: atmospheric entry, hypersonic flow, chemical reaction, ablation, ice, wind tunnel, CFD

Introduction

Frequent entries of extraterrestrial objects into the early earth's atmosphere are expected to have supplied the materials and energy necessary for forming the present earth [1]. Various chemical products in the high temperature shock layer flow over the ablating surface of an entry object were distributed into the atmosphere through the wake flow. In the present study, we consider the atmospheric entry of an icy object, because the water is one of the most common materials in the universe and it seems reasonable that such entry objects were mainly composed of the water ice. The Navier-Stokes analyses with the thermo-chemical nonequilibrium of the C-H-O-N 28 species show that Hydrogen Cyanide (HCN), which is one of the most important prebiotic materials, is efficiently produced near the surface in the stagnation region of an icy object entering the early earth's CO_2/N_2 atmosphere with the ablation injection of H_2O, and is transported into the atmosphere behind the object in almost frozen chemistry [2]. HCN is known to be significantly related to the production of amino acids. For example, adenine $C_5H_5N_5$, which is one of the bases of DNA [1], can be formed from 5 HCN's. If HCN had been efficiently produced in the high-temperature shock layer flow over ablating icy objects and supplied to the atmosphere through their wake flows, HCN from the hypersonic flow may have augmented the formation of biomolecules on the early earth.

To observe the behavior of an ice piece in hypersonic flow, the experimental studies have been conducted by the authors' research group at the hypersonic and high-enthalpy wind tunnel of Graduate School of Frontier Sciences, the University of Tokyo [3,4]. It was clearly seen that the ablation process with the phase change among vapor, water and ice at the surface plays an essential role in the phenomena of an icy object in hypersonic flow. When we put a spherical piece of water ice into the hypersonic flow at Mach number 7, the ice is melting in the stagnation region due to the severe aerodynamic heating and the surface recession significantly occurs there. On the other hand, in the shoulder region of the ice piece, the flow temperature rapidly decreases due to the strong expansion. Consequently, the vapor and/or liquid of water coming from the melting icy surface in the stagnation region are re-frozen into columns of solid ice there. The stack of such icy columns forms a complicated icy structure, which looks like the brim of a hat. As a result, the maximum diameter of the ice piece, as well as the drag force acting on it, is increasing with the exposure time in the flow until the fragmentation of icy columns due to the aerodynamic load. A typical image of such brim-like structure of ice is shown in the insert at the upper left corner of Fig. 1.

In the above process of the brim-like structure formation, a question arises: Which phase of water is transported from the stagnation region to the shoulder region, vapor (gas) or liquid? To answer to this question, we consider the phase diagram on the temperature-pressure plot shown in Fig. 1. In the experiment, the maximum available stagnation pressure (P0) and temperature (T0) are 0.95 MPa and 1000 K, respectively. The local pressure can vary from the order of 0.1 kPa (freestream condition level) to the order of 10 kPa (stagnation-point level), and the local temperature can vary from 70 K to 1000 K as indicated by a tinted area in the figure. As for the ablation process, the variation of the pressure and temperature on the surface is essential. To estimate the surface temperature of the ice piece, the use of the infrared (IR) camera is useful, because the water efficiently absorbs IR light and the black body model is applicable for water ice. A typical IR camera image is shown as an insert at the upper right corner of Fig. 1. We found that the surface temperature is kept in the range of 273-283 K during the exposure in the hypersonic flow thanks to the latent heat of the ablation. For measurement of the surface pressure over an ablating object, however, the efficient experimental technique is not available. To estimate the surface pressure, the CFD analysis of the Navier-Stokes equations is conducted for the body shape, which is determined from an instantaneous image of an ice piece in the flow as shown in the insert at the lower right corner of Fig. 1 [5]. In this case, the surface pressure is estimated to vary from 1kPa to 15 kPa. Finally we can indicate the variation of the temperature and pressure on the surface of the ablating ice piece in the flow of the hypersonic wind tunnel on the phase diagram as shown in Fig. 1. Under the assumption of the thermodynamic equilibrium, it is expected that the liquid water is transported over the surface from the stagnation region to the shoulder region. This may be a good example, in which the cooperation of CFD (Computational Fluid Dynamics) and EFD (Experimental Fluid Dynamics) can reveal the unknown mechanism of complicated phenomena.

The cooperation of CFD and EFD is also expected to play an important role in consideration of the chemical reaction process around an icy object entering the early earth’s atmosphere. The hypersonic wind tunnel is a very powerful tool to simulate and observe the shape change process due to ablation. As seen in the above, the process is too complicated to be simulated by the self-consistent CFD analysis, where both the shape change due to the ablation and the flow field around the body are simultaneously solved in a coupled manner. However, the ability of the wind tunnel facility to simulate the chemical reaction process around an icy entry object is quite limited. The impulse-type flow facility, such as a high-enthalpy shock tunnel, can produce gas flow at temperature high enough to excite the chemical reactions, but the test duration is too short to obtain the ablation around the body, which occurs in the time scale of seconds. On the other hand, the long duration facility like a blow-down-type wind tunnel can supply hypersonic flow for the test time long enough to observe the ablation process as shown in Fig. 1. However, the stagnation temperature is not high enough to excite the chemical reactions. In the present study, we have tried to use the hypersonic wind tunnel to simulate the chemical reactions around an icy entry body as well as its shape change due to ablation. To excite the chemical reactions in the flow of the hypersonic wind tunnel at the stagnation temperature less than 1000 K, the energy is locally added by the electric discharge. To develop such sophisticated experimental technique and to understand the obtained results, the cooperative approach of CFD and EFD is indispensable. In addition, the CFD analysis is necessary to predict the actual phenomena around an icy object at atmospheric entry from the phenomena observed in the hypersonic wind tunnel experiment.

The major objectives in the present study are 1) To consider the possible chemical reaction process of the HCN formation around an icy object entering the early earth’s atmosphere by the chemical nionequilibrium CFD analysis, 2) To predict the chemical reaction phenomena around an ice piece in the hypersonic wind tunnel flow with local energy addition by the electric discharge, 3) To design the experimental model based on the CFD results, and 4) To assess the usefulness of such experimental technique to simulate the chemical reactions in relation to the formation of the prebiotic materials around an icy entry object by the comparison between the CFD and EFD results.

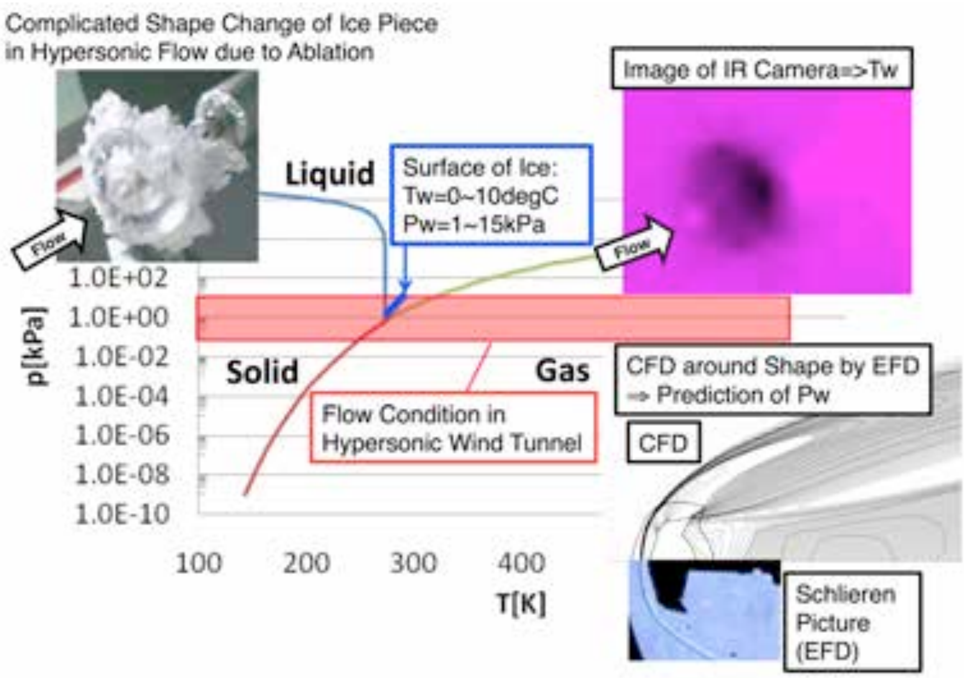

Fig. 1 Phase Diagram of Water and Ablation Process of Ice Piece in Hypersonic Wind Tunnel Flow

Chemical Reaction Process of Prebiotic Materials Formation around Icy Object

In this chapter, the chemical process of the production of HCN around an icy object entering the early earth's atmosphere and the results of the numerical analysis solving the Navier-Stokes equations with the nonequilibrium chemistry are briefly summarized based on Ref. [2].

The atmosphere of the early earth is thought to be similar to that of Mars of today and mainly composed of CO_2 and N_2. The chemical species to be considered for the hypersonic flow in the early earth's atmosphere with the ablation injection of H_2O from the icy surface of an extraterrestrial entry object will be almost the same as those to be considered for the hypersonic flow in the air (N_2 and O_2) with the gas injection from the CFRP ablator of the re-entry vehicle. Consequently, the chemical reaction model for the analysis of the ablator can be also used for the present study with small modification. The chemical reactions considered here consist of those of the 11-air-species (N_2, O_2, N, O, NO, NO^+, e^-, N^+, O^+, N_2^+, O_2^+) model, the reactions related to the carbon-containing species (C, C_2, C_3, CO_2, CO, CN, CO^+, C^+) and those of the carbon-nitrogen-oxygen-hydrogen species (H, H_2, HCN, HCO, C_2H_2, C_2H, CH, H_2O, OH). The detail is given in Ref. [2]. The thermal nonequilibrium is also considered with the two-temperature model of the translational-rotational temperature (T) and the vibrational-electronic-elctron temperature (T_v). The hybrid form of the conservative and nonconservative form equations for the axi-symmetric Navier-Stokes equation with the thermal and chemical nonequilibirum are numerically solved by using the symmetric TVD scheme for the convective terms. The non-conservative form equations are used for the nonequilibirum quantities, that is, the vibrational temperature and the mass fractions of the chemical species, because there is no discontinuity across the shock wave for these quantities.

In the present study, the ablation injection at the surface must be considered. Assuming that the surface of ice is non-catalytic, the mass fraction of the i-th species is determined by Eq. (1) that describes the mass conservation at the surface:

$$-D\frac{\partial C_i}{\partial n}+\rho\, C_i\, v_w = J_i\ , \tag{1}$$

where C_i, D, ρ, v_w and J_i are the mass fraction of the i-th species, the diffusion coefficient, the density of gas mixture, the injection velocity and the ablation injection rate of the i-th species, respectively. The outward normal velocity at the wall is calculated as:

$$v_w = (\sum_i J_i)/\rho_w\ . \tag{2}$$

The process of the HCN production is schematically illustrated in Fig. 2. In the present model, HCN is produced only by the reaction of CN and H_2. CN is supplied by the reactions involving the species in the freestream. H_2 is supplied by the reactions from H_2O. Consequently, HCN is expected to be produced in the vicinity of the wall in the forebody region, where the flow temperature is high enough to excite the chemical reactions. For HCN produced in the stagnation region to remain in the downstream region including the wake flow, the frozen chemistry must be sustained both in the shoulder region and in the wake region.

Figure 3 shows the typical results of the mass fraction of HCN around an icy entry object. The velocity and altitude are 8 km/s and 60 km, respectively. The atmospheric properties of the early Earth are assumed to be the same as those at present except the freestream composition as CO_2:N_2=0.93:0.07 by mass. The nose radius is 0.2m. The wall temperature is 273 K and the ablation injection rate of H_2O is uniform only on the forebody surface at 0.05 kg/m^2s. The upper half in the figure is the result of the laminar flow calculation, and the lower half is the result of the turbulent wake with the empirical mixing length model [6] and the turbulent Lewis number of 1.0. The computation is done on the 101X101 grid. Considering the pattern of the contour lines in Fig. 3, the main source of HCN exists in the vicinity of the surface in the stagnation region, and HCN spreads downstream by the advection and diffusion. To evaluate the extent of HCN production, the HCN production efficiency is defined as the ratio of the mass flux of HCN flowing out of the computational domain to the total ablation injection rate over the surface. In this case, the HCN production efficiency is 1.7×10^{-4}, which means the loss of an icy entry object of volume 1 m^3 results in the HCN production in the order of 0.1 kg. This number is not negligible. In Fig. 3, we assume a spherical icy object. As seen in the hypersonic wind tunnel experiments (Fig. 1), however, the shape after ablation is quite complicated, though the initial shape is sphere. To investigate the effect of the instantaneous shape of the ablating icy object on the chemical reaction, the CFD analysis is conducted for the forebody with the non-smooth shape as shown in Fig. 4. The freestream and ablation injection conditions are the same as in Fig.3. The result shows that the HCN production efficiency is hardly affected by the shape of the body.

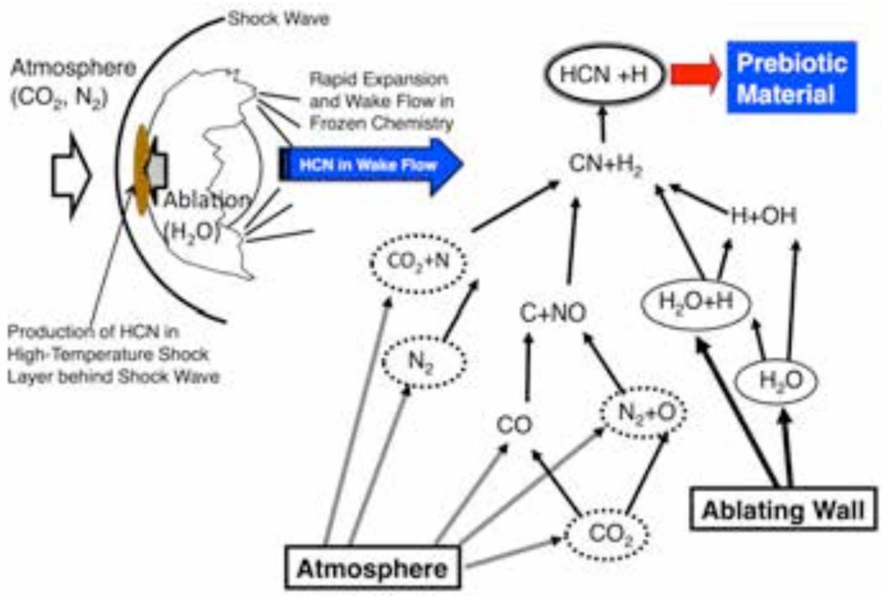

Fig. 2 Chemical Reaction Process of HCN Production in the Present Analysis Model

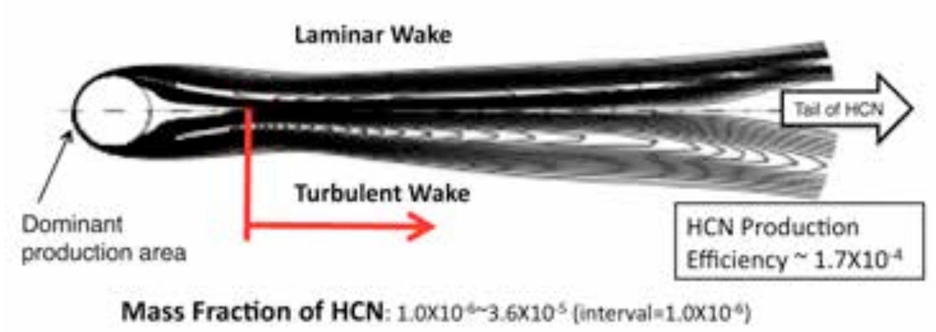

Fig. 3 Typical CFD Result on HCN Production

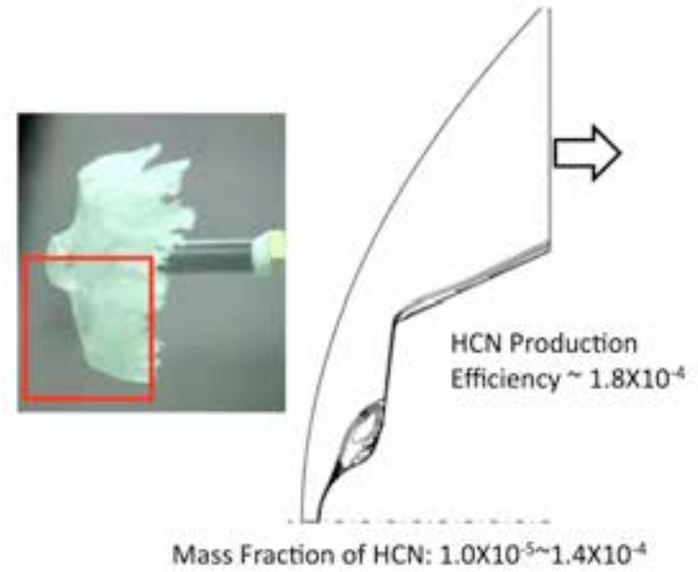

Fig. 4 CFD Results of HCN Production over Icy Body with Non-smooth Shape

Design of Experimental Model

Based on the results of the CFD analyses, the reasonable setup of the experimental apparatus is discussed in this chapter. The experiments are carried out at the hypersonic and high enthalpy wind tunnel in Kashiwa campus, the University of Tokyo [7]. The maximum available stagnation temperature (T0) and pressure (P0) are about 1000 K and 0.95 MPa, respectively. The diameter of the nozzle exit is 200 mm, and the uniform flow at Mach number 7.0-7.1 is obtained in the region with 120 mm diameter around the nozzle axis. In the case of a spherical model, the maximum diameter is limited to about 40 mm due to the blockage of the flow. When the hot shut-off valve opens, the flow starts, and the model is injected into the flow after the quasi-steady flow condition has been settled. Due to the nature of the pebble-bed-type heater installed in this facility, the stagnation temperature still continues to increase gradually at slow rate of 1 K/s. The maximum available test time is about 60 s after the hot shut-off valve opens.

The extent of the chemical nonequilibirum is evaluated well by the binary scaling parameter, which is defined as the product of the freestream density and the reference length [8]. In the present cases, the reference length is the diameter of an icy object. Figure 5 shows the variations of the binary scaling parameter with the altitude for various diameters. The range of the binary scaling parameter available in the wind tunnel is also indicated by the tinted area in the figure. The experimental flow condition here is equivalent to the atmospheric flight of an entry object with 0.1-1 m diameter at 50-70 km altitude, where the significant thermo-chemical nonequilibrium is expected.

To discuss the appropriate location of the energy addition by the electric discharge, the CFD analyses explained in the previous chapter have been made, assuming the laminar axi-symmetric flow. In the case of the early earth's atmosphere, the freestream composition is the mixture of CO_2 and N_2. In the wind tunnel experiment, however, the air (N_2 and O_2) is only available as the freestream composition. To simulate the production of HCN, some mechanism to supply the carbon and hydrogen elements must be intendedly installed. To supply C and H into the flow, we use the ablation of the experimental model. The shape of the experimental model is a hemispherical cylinder. The hemispherical nose is made from the mixture of dry ice and water ice. When the model is injected in to the hypersonic flow, the ablation occurs in the nose part and the carbon and hydrogen elements are automatically supplied into the flow of N_2 and O_2 by ablation. Consequently, the chemical reactions involving C, H, O, N elements including the production of HCN become possible. The after-body is made from non-ablative ceramic material and works as the model support having the circuit of the electric discharge in it. Because the effect of the nose shape on the production of HCN is not so significant as seen in Fig. 4, a simple hemispherical shape is selected for the nose of the model.

First, we assume the electric discharge in the stagnation region, where the flow is slow and various chemical reactions are expected to be excited. The 161X171 grid for the CFD study is shown in Fig. 6. Figures 7 and 8 show the result of the CFD analysis. The freestream Mach number, P0 and T0 are 7.0, 0.95 MPa and 1000 K, respectively. The energy addition by the electric discharge is described by the source term in the equation of the viblational temperature. After the energy of the electric discharge is absorbed in the vibrational mode, the translational temperature will be raised by the translational-vibrational energy exchange. The uniform energy addition is assumed in the very thin region with 5 mm diameter around the model axis and the thickness of 1 mm from the surface, because the Joule heating of the electric discharge is expected to be confined in the sheath region. In this case, the total heat input is 500 W, which is available by the power source used in the experiment, and the density of the energy addition is 7×10^9 W/m^3. The uniform ablation injection is assumed at 0.1 kg/m^{2}s over the hemispherical nose. The mixture ratio is CO_2:H_2O=1:1 by mass. No ablation occurs in the region of the energy addition, because the electrodes are placed there. The distributions of the translational and vibrational temperatures are shown in Fig. 7. The maximum vibrational temperature is estimated as about 8800 K in the stagnation region. That is high enough to excite the chemical reactions of C, H, O and N. On the other hand, the translational temperature is much smaller than the vibrational temperature. Figure 8 shows the distribution of the mass fraction of HCN. In this case, the production of HCN is negligible, because the ablation injection occurs in the downstream of the energy addition, and the C and H elements are supplied to the region of high vibrational temperature only by the diffusion. Consequently, the stagnation region is not appropriate for the place of the electric discharge.

Based on the above discussion, the design of the experimental model is determined as shown in Fig. 9. The body is composed of two parts: The nose part is made from the mixture of water ice and dry ice in the hemispherical mold. The rear part is made from ceramic. The electric discharge circuit is designed based on our previous study on the plasma discharge on a flat plate [9, 10]. On the side surface, the electrodes are installed as shown in the figure, and are connected to the power supply system. For stable electric discharge, the cathode is set upstream of the anode. The electric power system is a combination of the high power supply (max. 500V, max. 6A) and the high voltage one (max. 1kV, max. 200 mA). To stabilize the plasma discharge, the high voltage power supply is switched on to ignite the plasma discharge again, when the plasma becomes weak and the current drops. After the model is injected into the hypersonic flow, the ablation occurs over the surface of the nose part, and CO_2 and H_2O are injected into the flow. The ablation injection rate is estimated from the surface recession rate, which can be determined from the temporal variation of the nose shape captured by the video camera.

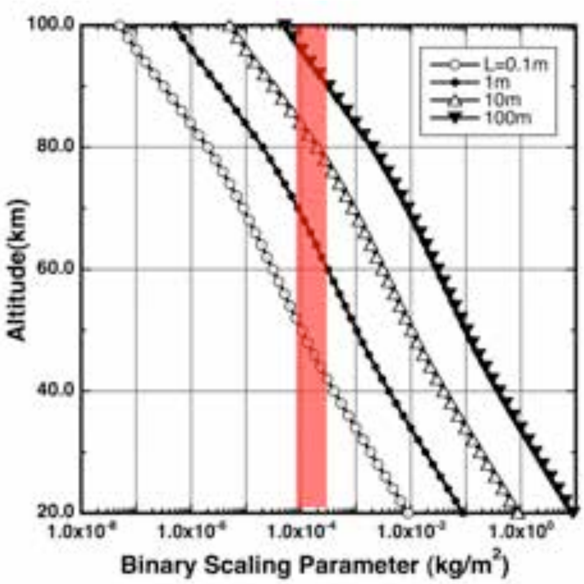

Fig. 5 Binary Scaling Parameter at Entry Flight and at Wind Tunnel Experiment

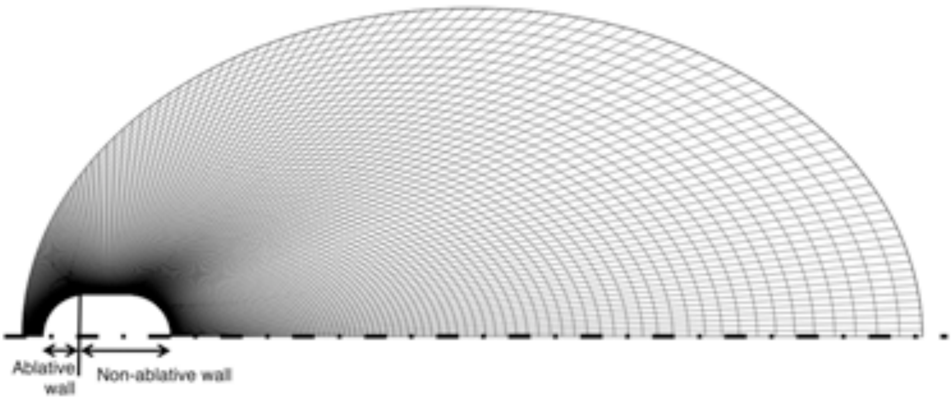

Fig. 6 Computational Grid for CFD Analysis

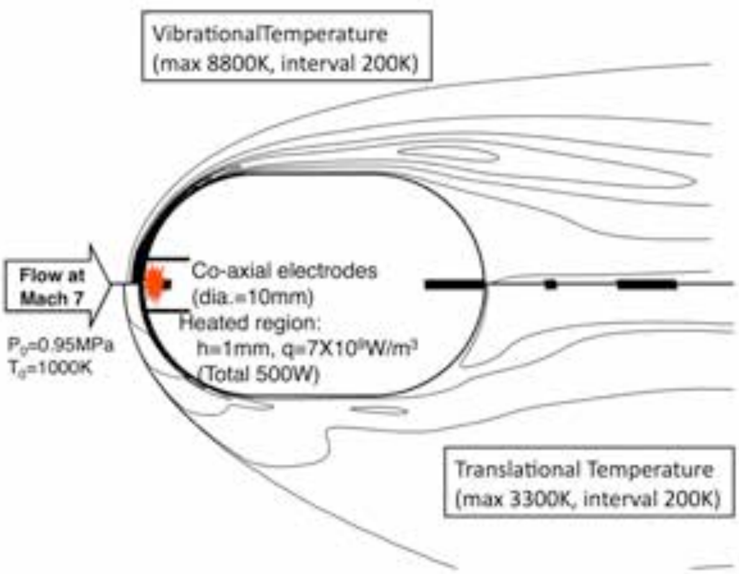

Fig. 7 Translational and Vibrational Temperatures by CFD in Case of Electric Discharge in Stagnation Region

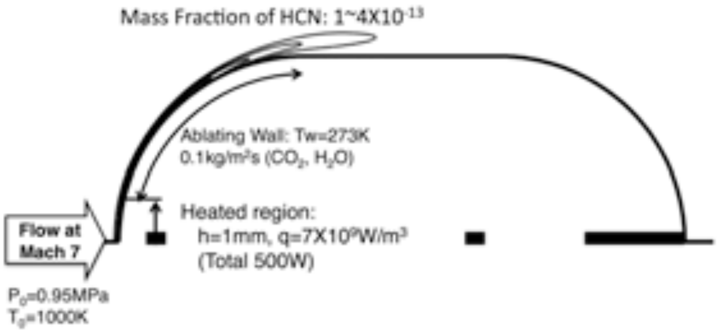

Fig. 8 Mass Fraction of HCN by CFD in Case of Electric Discharge in Stagnation Region

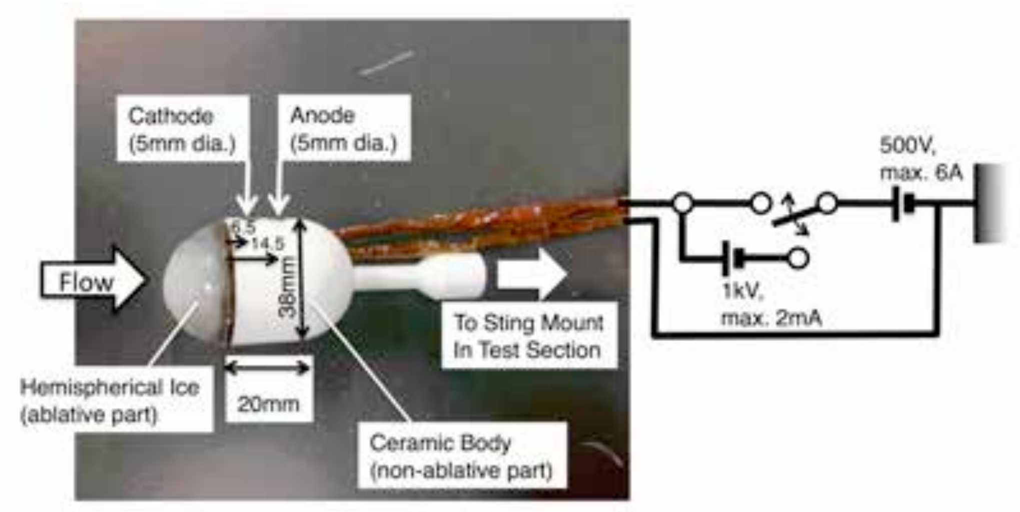

Fig. 9 Experimental Model with Electric Discharge on Side Surface

Results and Discussion

Using the experimental model shown in Fig. 9, the hypersonic wind tunnel experiment was carried out. Figure 10 shows the snapshots of the normal video and schlieren video. Strong light emission is seen around the location of the electric discharge. P0 and T0 of the flow are 950 kPA and 600-650 K, respectively. The input power is about 100 W. When the stable discharge has been established, the voltage between the cathode and anode drops to 10-20 V. The nose part is made from the mixture of water ice and dry ice. From the recession rate of the nose surface taken by the video camera, the ablation injection rates of H_2O and CO_2 are roughly estimated as 0.05 kg/m^{2}s and 0.05 kg/m^{2}s, respectively. It should be noted that the shock wave shape in the schlieren image seems almost symmetric with respect to the centerline, though the discharge occurs only on the upper side. In this case, the energy addition by the electric discharge hardly affects the formation of the shock wave.

To deepen our understanding on the phenomena seen in Fig. 10, especially from a viewpoint of the chemical reactions, the thermo-chemical nonequilibirum CFD analysis has been conducted. Though the phenomena in the experiment are three-dimensional due to the arrangement of the electrodes, we assume the axi-symmetric flow as the preliminary analysis. The pressure distribution of the CFD result is shown in Fig. 11. The zone of energy addition is set on the cylindrical part of the body. The input power density is uniform at 3X10^{9}W/m^3. This is equivalent to the heat input of 100 W in a region of 3mm width, 1mm height and 10 mm length. It is confirmed by the CFD that the shock wave shape is hardly affected by the energy addition. Figure 12 shows the distributions of the translational temperature and vibrational temperature. The vibrational energy of the flow is excited up to 12500 K in the vicinity of the electric discharge. The translational temperature is also raised up to 4000 K by the translational-vibrational energy exchange there. These values are in the same order as in the stagnation region at the actual atmospheric entry flight. Various chemical reactions are expected in the discharge region in the similar way to the stagnation region of the entry object. Figure 13 shows the distributions of the mass fractions of CN and HCN. Though their quantities are quite small, the CFD result indicates that these species will be formed over the region of the electric discharge and remain in the downstream flow.

From a viewpoint of the possibility of the prebiotic materials formation in high temperature shock layer flows, the presence of HCN should be directly confirmed in the wind tunnel flow. Unfortunately, HCN does not have the light emission of the wavelength in the visible range. In the present study, we observe the light emission of CN, because CN is a reactant of the production of HCN as shown in Fig. 2. The image through the band pass filter of 382-398 nm, which includes the wavelength of the light emission of CN, is shown in an insert of Fig. 14. The presence of the luminous spot indicates the formation of CN there, and, as a result, suggests the formation of HCN in the hypersonic flow. In general, the intensity of the emission becomes stronger in the region at higher vibrational temperature and larger number density of the species. Roughly speaking, the intensity of the emission from CN will be in proportion to $I = T^m T_v^n \rho_{CN}$. The contour lines of I from the CFD result are shown in the lower half of Fig. 14. The exponent m and n are set as 0 and 4, respectively. A similar pattern is obtained in comparison with the experimental image through the band pass filter. Consequently, the presence of CN in the flow is also supported by the CFD. Of course, the present discussion is based on very rough model for the phenomena. For further consideration, more precise heat input model for the electric discharge, detailed computational radiation emission analysis based on the line-by-line method, consideration of the three-dimensionality of the phenomena and so on are necessary.

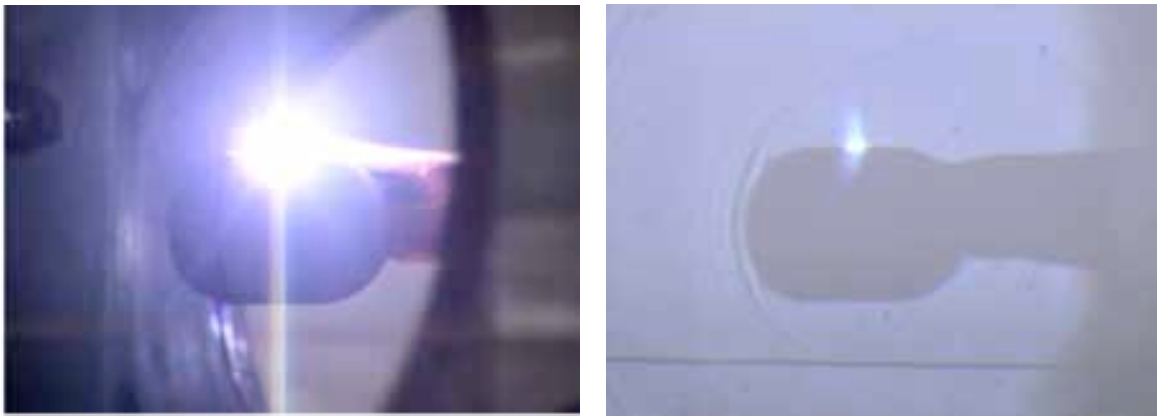

Fig. 10 Snapshots of Normal Video (left) and Schlieren Video (right) of Model in Hypersonic Flow with Electric Discharge

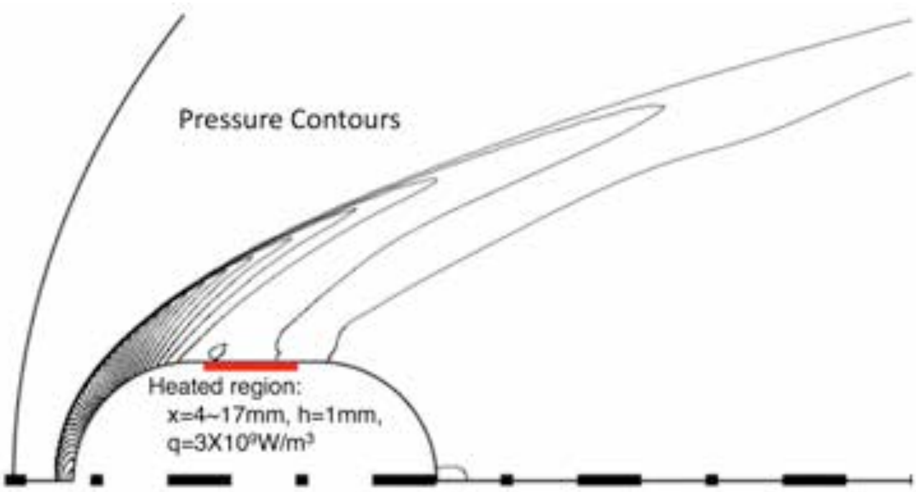

Fig. 11 Pressure Distribution by CFD for Experimental Condition

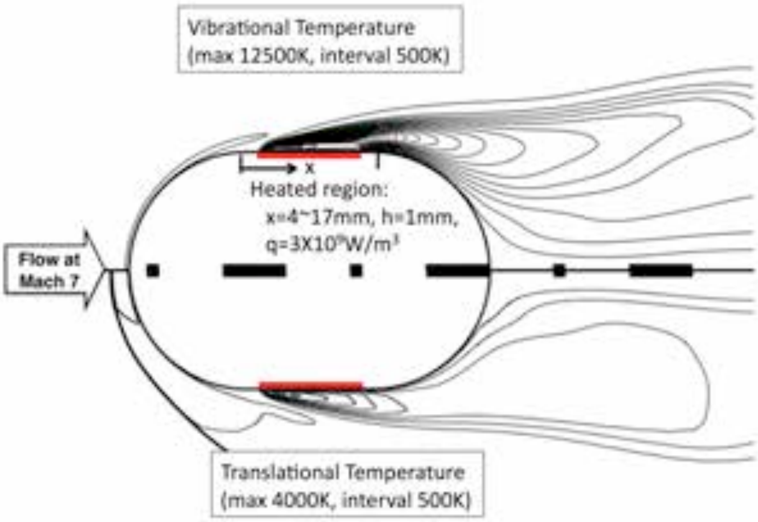

Fig. 12 Translational and Vibrational Temperatures by CFD for Experimental Condition

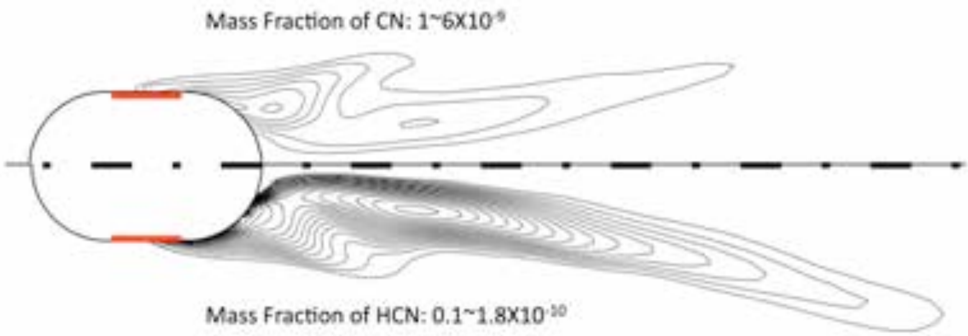

Fig. 13 Mass Fraction of HCN and CN by CFD for Experimental Condition

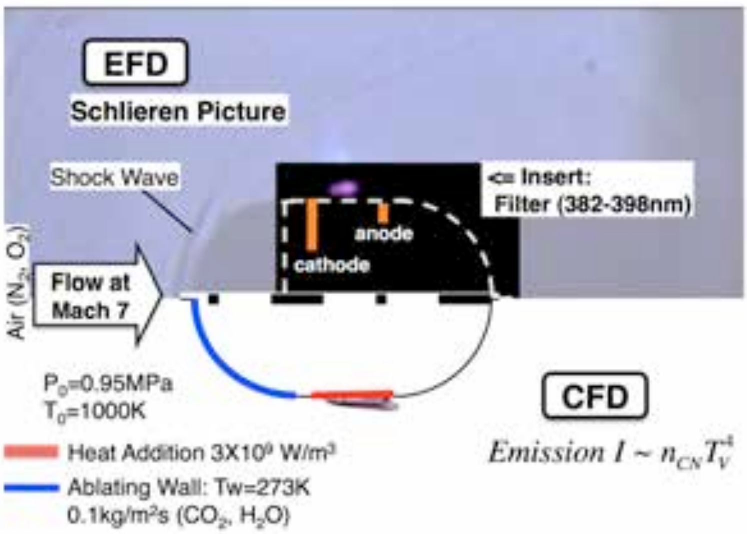

Fig. 14 Comparison between Experimental Picture of CN Emission and Estimation by CFD

Concluding Remarks

Frequent entries of extraterrestrial objects into the early earth's atmosphere are expected to have supplied the materials and energy necessary for forming the present earth. Various chemical products in the high temperature shock layer flow over the ablating surface of an entry object were distributed into the atmosphere through the wake flow. The Navier-Stokes analyses with the thermo-chemical nonequilibrium of the C-H-O-N 28 species show: 1) HCN, which is one of the most important prebiotic materials, is efficiently produced near the surface in the stagnation region of an icy object entering the early earth's CO_2/N_2 atmosphere with the ablation injection of H_2O, and 2) HCN is transported into the atmosphere by the wake flow behind the object with almost frozen chemistry. To simulate experimentally such process in the hypersonic wind tunnel with relatively low stagnation temperature, the energy addition technique by the electric discharge is proposed. The C and H elements are supplied by the ablation injection at the body surface made from the mixture of water ice and dry ice. The experimental model consists of two parts: ablative nose part to supply the C and H elements and the non-ablative after-body, in which the circuit of the electric discharge is installed in it to supply the energy necessary for chemical reactions. To predict the chemical reaction phenomena around the model in the flow of the hypersonic wind tunnel, the thermo-chemical nonequilibrium CFD analysis has been conducted. Based on the CFD results, the location of the electrodes for the electric discharge is determined to be in the downstream of the ablative nose part. The light emission of CN is experimentally observed through the band pass filter. A similar spatial distribution of the emission of CN is reproduced in the CFD result. Consequently, the cooperative approach of the EFD and CFD will deepen our understanding on the chemical process around an extraterrestrial objects entering the earth's atmosphere in the period of the heavy bombardment $4\text{-}3.8 \times 10^9$ years ago.

Acknowledgments

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