Hydrodynamical-Chemical Models from Prestellar Cores to Protostellar Cores

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Abstract. We investigate the molecular evolution in star forming cores from dense cloud cores ($n_H \sim 10^4$ cm^{-3}, $T \sim 10$ K) to protostellar cores. A detailed gas-grain reaction network is solved in infalling fluid parcels in 1-D radiation hydrodynamic model. Large organic molecules are mainly formed via grain-surface reaction at $T \sim$ several 10 K and sublimated to the gas-phase at ~ 100 K, while carbon-chain species are formed at a few 10 K after the sublimation of CH$_4$ ice. The former accounts for the high abundance of large organic molecules in hot corinos such as IRAS16293, and the latter accounts for the carbon chain species observed toward L1527. The relative abundance of carbon chain species and large organic species would depend on the collapse time scale and/or temperature in the dense core stage. The large organic molecules and carbon chains in the protostellar cores are heavily deuterated; although they are formed in the warm temperatures, their ingredients have high D/H ratios, which are set in the cold core phase and isothermal collapse phase. HCOOH is formed by the gas-phase reaction of OH with the sublimated H$_2$CO, and is further enriched in Deuterium due to the exothermic exchange reaction of OH + D → OD + H.

In the fluid parcels of the 1-D collapse model, warm temperature $T \sim$ several 10 K lasts for only $\sim 10^4$ yr, and the fluid parcels fall to the central star in ~ 100 yr after the temperature of the parcel rises to $T \geqslant 100$ K. These timescales are determined by the size of the warm region and infall ($\sim$ free-fall) velocity: r_{warm}/t_{ff}. In reality, circum stellar disk is formed, in which fluid parcels stay for a longer timescale than the infall timescale. We investigate the molecular evolution in the disk by simply assuming that a fluid parcel stays at a constant temperature and density (i.e. a fixed disk radius) for $10^4 - 10^5$ yrs. We found that some organic species which are underestimated in our 1-D collapse model, such as CH$_3$OCH$_3$ and HCOOCH$_3$, become abundant in the disk. We also found that these disk species have very high D/H ratio as well, since their ingredients are highly deuterated.

Finally we investigate molecular evolution in a 3D hydrodynamic simulation of star forming core. We found CH$_3$OH are abundant in the vicinity of the first core. The abundances of large organic species are determined mainly by the local temperature (sublimation), because of the short lifetime of the first core and the efficient mass accretion via angular momentum transfer.

Keywords. stars: formation, ISM: clouds, ISM: abundances

1. Introduction: Hydro-Chemical Models

In star-forming cores, temperature and density vary temporally and spatially. Major chemical processes, which determine the molecular abundances in these cores, also change according to the physical conditions. In prestellar cores with high densities and low temperatures, various molecules are depleted onto grains, where they are hydrogenated by grain-surface reactions. In protostellar phase, on the other hand, molecules are desorbed

to the gas phase in the central high-temperature regions. The molecular abundances in the star-forming cores thus change dramatically in the course of the star formation.

It is also well established that molecular clouds are generally not in chemical equilibrium; chemical timescale is comparable or longer than the dynamical timescale of the clouds. For example, the adsorption timescale of gaseous species onto grain surfaces in cold prestellar cores is

$$\pi a^2 \sqrt{\frac{8kT}{\pi m}} S n_{\mathrm{grain}} \sim 1 \times 10^6 \left(\frac{10^4 \mathrm{cm}^{-3}}{n_{\mathrm{H}}} \right) \mathrm{[yr]}, \tag{1.1}$$

where a ($\sim 10^{-5}$ cm) and n_{grain} are the size and number density of the grain particles, respectively, and S(~ 1.0) is the sticking probability. It is comparable to the free-fall timescale of a cold core

$$t_{\mathrm{ff}} = \sqrt{\frac{3\pi}{32G\rho}} \sim 4.3 \times 10^5 \left(\frac{10^4 \mathrm{cm}^{-3}}{n_{\mathrm{H}}} \right)^{1/2} \mathrm{[yr]}. \tag{1.2}$$

We thus need hydro-chemical models in order to investigate molecular abundances and their spatial distribution in star forming cores theoretically.

In the hydro chemical models of star-forming cores, we solve the chemical reaction network (i.e. rate equations) in Lagrange fluid parcels. If the hydrodynamic models are calculated in the Eulerian coordinate, we follow the trajectories of Lagrangian parcels to get the temporal variation of physical parameters in the fluid parcels. The Lagrangian coordinate is more convenient than the Eulerian coordinate to understand the non-equilibrium chemistry, in which molecular abundances are determined not only by the local physical conditions but also by the temporal variation of physical parameters in the past.

In this article, we present hydro-chemical models of low-mass star forming cores. The models start from cold dense cores and evolve to protostellar cores. We first show a spherical core model, in which we calculate molecular abundances and D/H ratios in the gas phase and ice mantles. Then we briefly discuss the chemistry in circum stellar disks. Finally we present preliminary results of a 3-D hydro-chemical model of star-forming cores.
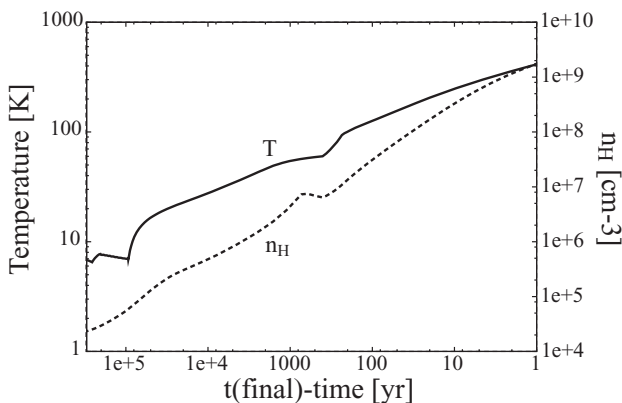

Figure 1. Temporal variation of density and temperature in the fluid parcel which falls from $r \sim 1 \times 10^4$ AU to 2.5 AU.

2. Spherical model

2.1. *Radiation hydrodynamic model*

Hydrodynamic evolution of star-forming cores have been extensively studied by numerical calculations for decades (Klein *et al.* 2007 and references therein). There are also well known semi-analytical models such as Larson-Penston collapse (Larson 1969; Penston 1969) and inside-out collapse model (Shu 1977). But many of these models assume isothermal conditions or polytropes, and thus do not solve the energy equation for temperatures, which is critically important for chemistry. For hydro-chemical models we need radiation hydrodynamic models in which energy equations are solved.

Here we adopt the 1D (spherical) radiation hydrodynamic model of a low-mass star formation by Masunaga *et al.* (1998) and Masunaga & Inutsuka (2000) (Aikawa *et al.* 2008). Initially, the central density of the dense prestellar core is $\rho = 1.4 \times 10^{-19}$ g cm^{-3}, which corresponds to a number density of hydrogen nuclei $n_H \sim 6 \times 10^4$ cm^{-3}. The contraction is almost isothermal as long as the cooling rate overwhelms the compressional heating, but eventually the latter dominates and the temperature rises in the central region. The model goes through the first core phase and the second collapse, and follows the evolution of the protostar up to the age of 9.3×10^4 yr.

Figure 1 shows the temporal variation of density and temperature in the fluid parcel which is initially at 1×10^4 AU and falls to 2.5 AU at the final step of the model. Naturally, the density and temperature increase with time. It is well known that the free-fall timescale of a isothermal sphere is proportional to $\rho^{-1/2}$. While the core temperature rises in the central region, the infall velocity accelerates toward the center until the fluid parcel hits the surface of central hydrostatic core (first core or protostar). Hence the temporal variation of density and temperature accelerate as well. In order to highlight the rapid rise near and at the final stage, the horizontal axis in Figure 1 is set to be the logarithm of $t(\text{final}) - t$, where $t(\text{final})$ corresponds to 9.3×10^4 yr after the birth of the protostar.

Temporal variation of temperature is critically important for chemistry. Garrod & Herbst (2006) show that the grain-surface reactions of heavy-element species are efficient in a limited temperature range: several 10 K. Once the temperature gets higher than ~ 100 K, most volatile species are sublimated to the gas phase, where they start the gas-phase reactions. In Figure 1, we can easily read the timescale of these warm phases; the fluid parcel stays at the temperature of several 10 K for slightly less than 10^4 yr. After the fluid parcel gets waremr than 100 K, it falls to the central star in a few 100 yr. Although these timescales slightly depend on the model parameters such as the initial mass of the core, they do not significantly difference from the value in Figure 1; the timescales are approximately equal to $r_{\text{warm}}/v_{\text{infall}}$, where r_{warm} is the size of the warm region, and the infall velocity v_{infall} is close to the free-fall velocity.

We solve the rate equations of the gas-grain reaction network of Garrod & Herbst (2006) along the temporal variation of the physical parameters in Figure 1. We have also extended the original model of Garrod & Herbst (2006) to include deuterated species referring to Millar *et al.* (1989) and Roberts *et al.* (2004) in order to investigate molecular D/H ratios. Here we assume that the dense core is initially supported by turbulence and/or magnetic fields; we calculate the reaction network model under the cold cloud condition (T=10K, $n_H \sim 10^4$ cm^{-3}) for 1×10^6 yr before we adopt the temporal variation of physical parameters in Figure 1. By performing similar calculations for various infalling fluid parcels, we can obtain radial distribution of molecular abundances in the protostellar core.

2.2. *Molecular Abundances in the Protostellar Core*

Figure 2 shows the radial distribution of physical parameters and molecular abundances in the protostellar core of age 9.3×10^4 yr. Many molecules (e.g. NH_3, H_2O and large organic molecules) are sublimated to the gas-phase at $r \sim 100$ AU, where temperature reaches ~ 100 K. The ionization degree decreases toward the center, because it is proportional to $n_H^{-1/2}$. In the outer part of the envelope ($r \geqslant 1000$ AU) HCO^+ is the dominant positive ion. In the inner regions, on the other hand, molecules with higher proton affinities than CO are sublimated. There, the dominant ions are H_3CO^+ and NH_4^+.

Methanol and H_2CO ices are abundant out to 10^4 AU, which indicates that they are formed even in the molecular cloud conditions ($T \sim 10$ K) (Figure 2c). Other large organic molecules (both in the gas phase and ice mantle), on the other hand, are abundant only inside a few 1000 AU; they are formed by the grain surfaces reactions among heavy element species at warm temperature ($T \sim 40$ K) and the gas-phase reactions of sublimated species such as H_2CO (Garrod & Herbst 2006; Aikawa *et al.* 2008). The large organic species are sublimated to be observed as hot corinos (e.g. Ceccarelli. *et al.* 2007)

Figure 2(d) shows the distribution of carbon chain species. They increases toward the center at $r \sim 1000$ AU, where CH_4 is sublimated to the gas phase and partly converted to these carbon chains via gas-phase reactions (Sakai *et al.* 2008; Aikawa *et al.* 2008; Hassel *et al.* 2009). It is observed as warm carbon chain chemistry (WCCC) (see Sakai *et al.* in this volume).

It is worth noticing that both hot corino species and WCCC species are formed in our model. In observations, on the other hand, the carbon chains are not abundant in Hot Corinos, and the large organic molecules are not abundant in WCCC objects (Sakai *et al.* 2009). It should depend on the initial ice abundance of CH_3OH and CH_4, which are formed in the cold prestellar phase (Sakai *et al.* 2009). Aikawa *et al.* (2005) investigated
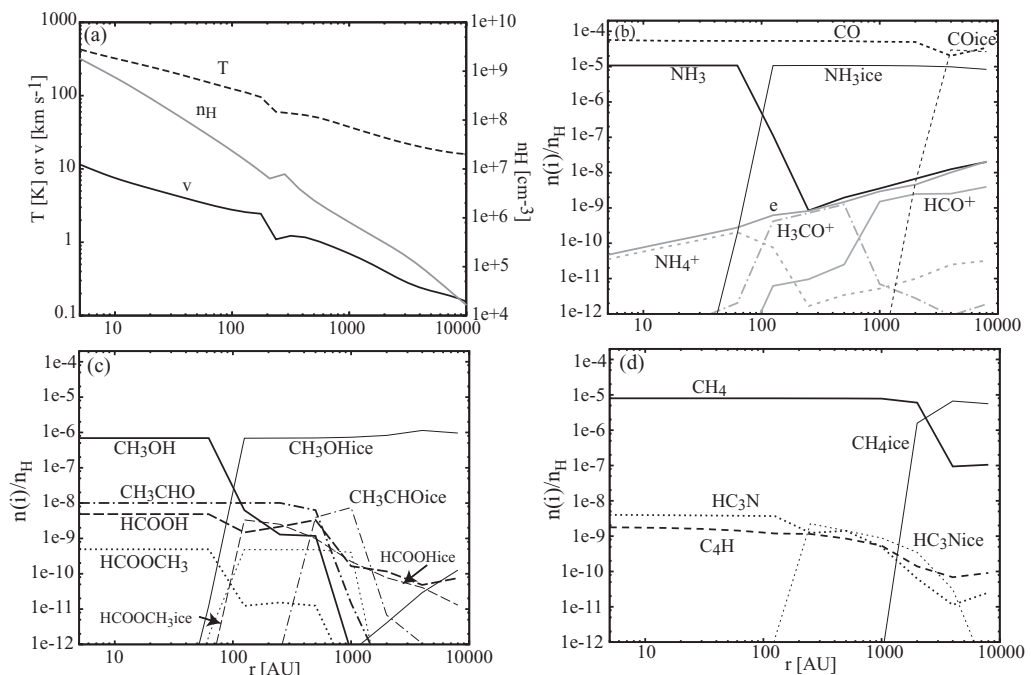

Figure 2. Distribution of (a) physical parameters and (b-d) molecular abundances in the protostellar core of age 9.3×10^4 yr.

gas-grain chemistry in isothermal (cold) collapse phase and shows that CH_3OH is more abundant than CH_4 ice in the slow collapse model starting from near equilibrium conditions, while CH_4 ice is more abundant in the model of faster collapse with a smaller pressure/gravity ratio. The abundance of CH_3OH ice and CH_4 ice may also depend on the temperature in the cold phase, i.e. whether it is slightly higher or lower than 10 K.

2.3. *D/H ratios*

Figure 3 shows the temporal variation of deuterated species and their normal isotope counterparts in the fluid parcel falling to 2.5 AU. In the cold phase, molecules are enriched with Deuterium due to the exothermic exchange reactions such as $H_3^+ + HD \rightarrow H_2D^+ + H_2$. Although such exothermic exchange reactions are limited to several species (Millar *et al.* 1989), the high D/H ratio propagates to other molecules via gas-phase reactions and grain-surface reactions. For example, H_2D^+ gives its deuteron to other molecules and atoms via ion-molecule reactions. H_2D^+ also recombines to produce D atom, which are adsorbed onto grains and hydrogenate the ice mantle species. Once the core gets warm, H_2D^+ is rapidly destroyed by the endothermic exchange reaction with H_2. But deuterated neutral species are not easily destroyed (ex. CH_3D in Figure 3a). Large organic molecules and warm carbon chains, which are formed at warm temperatures, also have high D/H ratios, because they are formed from molecules with high D/H ratios. In our model, DCOOH/HCOOH ratio is further enhanced at $t(\text{final})$-$t \sim$ a few 10^3 yr. HCOOH is formed by the reaction of sublimated H_2CO with OH, which is deuterated by the exchange reaction $OH + D \rightarrow OD + H$ with high exothermicity ($\Delta E \sim 810$ K.)

3. Circumstellar disk

So far, we adopted a spherical symmetric model of star-forming cores. In the spherical model, fluid parcels fall to the central star in a short timescale (~ 100 yr), once they enter the region of $T \geqslant 100$ K (Figure 1). But in reality, dense cores are rotating ($\omega \sim 10^{-14}$ s^{-1}), and the spherical symmetry breaks in the central regions as the collapse proceeds. Because of the angular momentum conservation, the centrifugal force increases for infalling fluid parcels and eventually balances with the gravity at the centrifugal radius

$$r_{\text{cent}} = \frac{(r^2\omega)^2_{\text{init}}}{GM} \sim 400 \left(\frac{r}{0.1\text{pc}}\right)^4 \left(\frac{\omega}{1 \times 10^{-14}\text{s}^{-1}}\right)^2 \left(\frac{1M_\odot}{M}\right) \text{AU} \qquad (3.1)$$

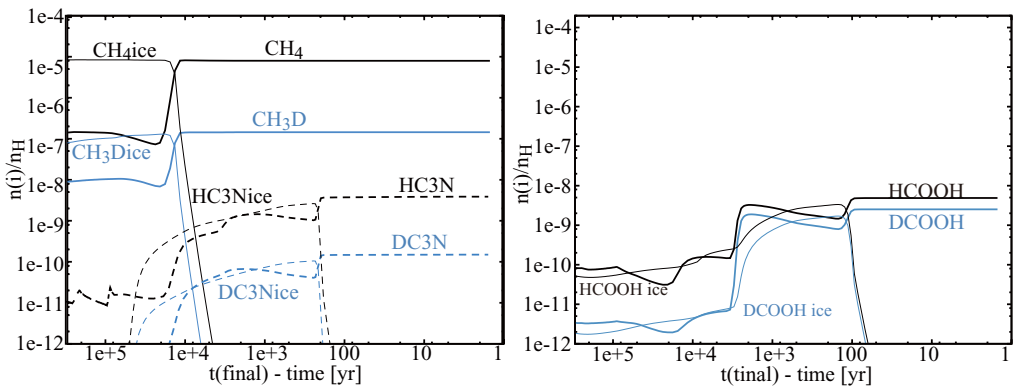**Figure 3.** Temporal variation of deuterated molecules and thier normal isotope counterparts in the fluid parcel falling to $r = 2.5$ AU. The horizon axis is the same as that of Figure 1.

to form a circumstellar disk. It means that the fluid parcels stay in the warm dense regions for a longer time scale than assumed in the spherical model. In order to investigate the chemistry in this prolonged warm phase, we performed a pseudo time dependent model (i.e. fixed density and temperature). As the initial abundances, we adopt the molecular abundances at 2.5 AU in final step of the spherical collapse model.

Figure 4 shows the temporal variation of molecular abundances at (a) $T = 260$ K and (b) $T = 40$ K. The density is set to be $n_H = 4 \times 10^8$ cm^{-3}. We can see that significant amount of gaseous CH$_3$OCH$_3$ and HCOOCH$_3$ ice are formed in $10^4 - 10^5$ yr via gas-phase reactions and grain-surface reactions, respectively. It should be noted that the abundances of these species are underestimated in our spherical model ($n(CH_3OCH_3)/n_H = 2 \times 10^{-11}$ and $n(HCOOCH_3)/n_H = 5 \times 10^{-10}$ inside $r \sim 100$ AU) compared with the estimated abundances in the observations: $n(CH_3OCH_3)/n_H \sim 10^{-7}$ and $n(HCOOCH_3)/n_H \sim 10^{-9} - 10^{-7}$ (Cazaux *et al.* 2003; Chandler *et al.* 2005; Kuan *et al.* 2004). It indicates that hot corinos are composed of the envelope and the circumstellar disk, and some species (e.g. H$_2$CO and CH$_3$CHO) are abundant in the envelope, while others (e.g. CH$_3$OCH$_3$) are abundant in the disk regions. Observations with a high spatial resolution is needed to confirm this prediction.

It should also be noted that the D/H ratio of CH$_3$OCH$_3$ are a few %, inspite of its formation at 260 K (Figure 4*a*). Again, the high D/H ratio is a relic of the low-temperature chemistry; CH$_3$OCH$_3$ is formed from molecules (e.g. CH$_3$OH) with high D/H ratios, which are set in the cold phase.

4. 3D model of the first core formation

4.1. *the physical model and trajectories*

In order to understand the chemistry in star-forming cores with disks more quantitatively, it is necessary to adopt 2D or 3D models. Semi-analytical 2D model is presented in Visser *et al.* in this volume. Here we show preliminary results of chemistry in a 3D model, in which a cold dense core collapses to form the first core (Furuya *et al.* in prep). The first core is a transient hydrostatic core of H$_2$; after several 10^3 yrs, H$_2$ dissociates and the core collapses to form a protostar. In spite its short life time, it plays important roles in the star formation: (i) given a large amount of angular momentum, it can fragment to form a binary system (Matsumoto & Hanawa 2003), (ii) it drives an outflow (Tomisaka
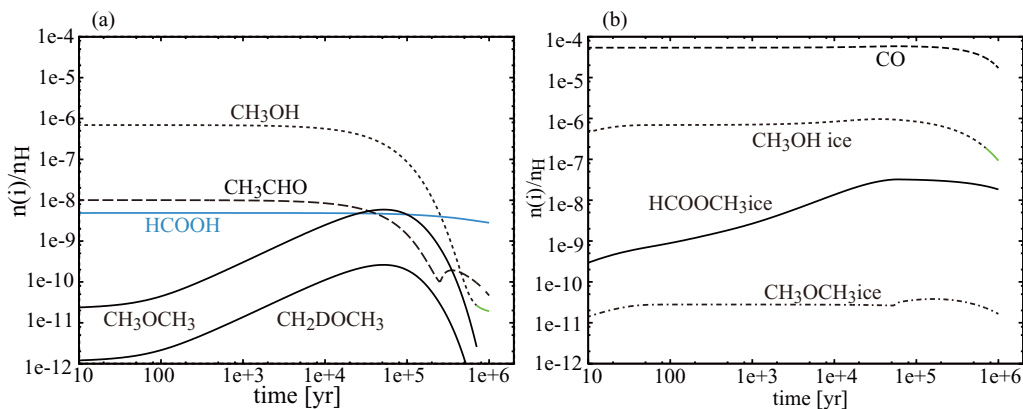

Figure 4. Temporal variation of molecular abundances at fixed temperatures and density after the fluid parcel enters the disk. The temperature is (a) $T = 260$ K and (b) $T = 40$ K, while the density is set to $n_H = 4 \times 10^8$ cm^{-3}.

2002) and (iii) outer part of the first core evolves to the protoplanetary disks (Machida *et al.* 2010).

We adopt the 3D radiation hydrodynamic model by Tomida *et al.* (2010); the model is based on the 3D nested grid code of Matsumoto & Hanawa (2003) and developed to include the radiation transfer with the gray flux-limited diffusion approximation. The central dense region is divided to finer grids to resolve the structure; the finest grid corresponds to 0.08 AU, while the size of the model core as a whole extends to ~ 0.1 pc. Figure 5(a) shows trajectories of three fluid parcels. In the envelope region, the trajectories are almost free-fall, until the parcels enter the disk in the central region. The temporal variation of physical parameters in the fluid parcels are shown in Figure 5(b).

Since the hydrodynamic model contains a wide range of density and temperature, we combine several chemical network models to follow the chemistry in the parcels. At low temperatures ($T \leqslant 100$ K), we adopt the gas-grain model of Garrod & Herbst (2006), while at the higher temperatures we adopt Harada *et al.* (2010). We also implemented collisional dissociations and three-body reactions, which can be important at high temperatures and high densities, respectively, referring to Willacy *et al.* (1998). Rate coefficients and activation barriers of some collisional dissociations are updated referring to NIST-Janaf Thermochemical Tables of the heat of formation. Grain charge is solved referring to Umebayashi (1983); while at low densities ($n_H \leqslant 10^{12}$ cm^{-3}) most of the grain particles are negatively charged and can be an important recombination partner of positive ions, neutral grains are dominant at higher densities.
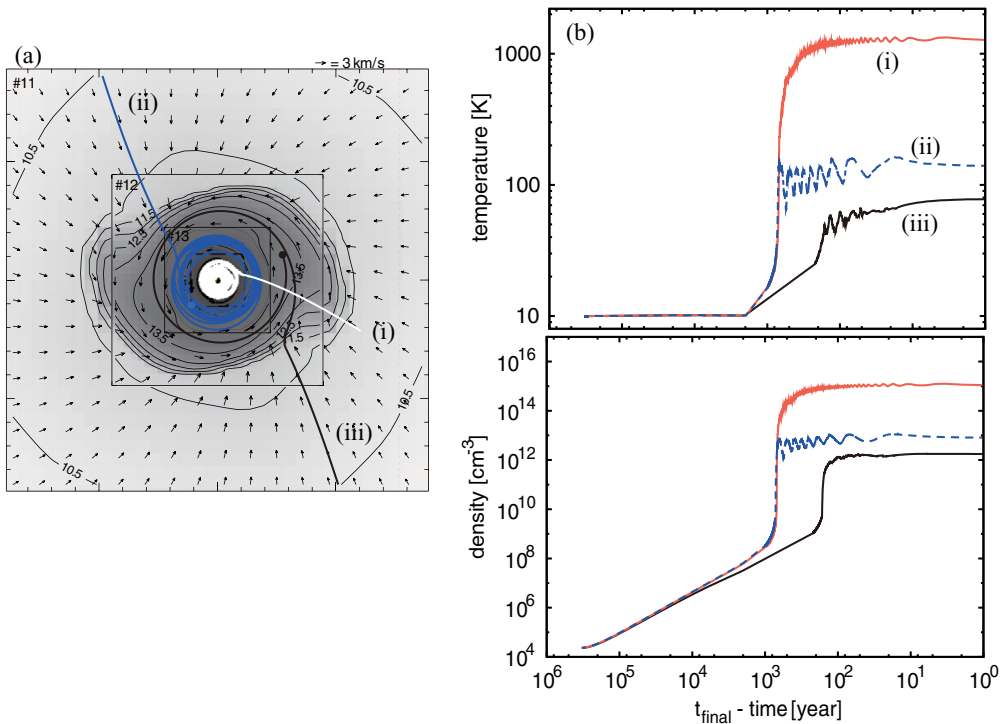

Figure 5. (a) Trajectories of the representative three fluid parcels in the 3D radiation hydrodynamic model. The counters depict the density distribution in the $z = 0$ plane. (b) Temporal variation of temperature and density in the three fluid parcels.
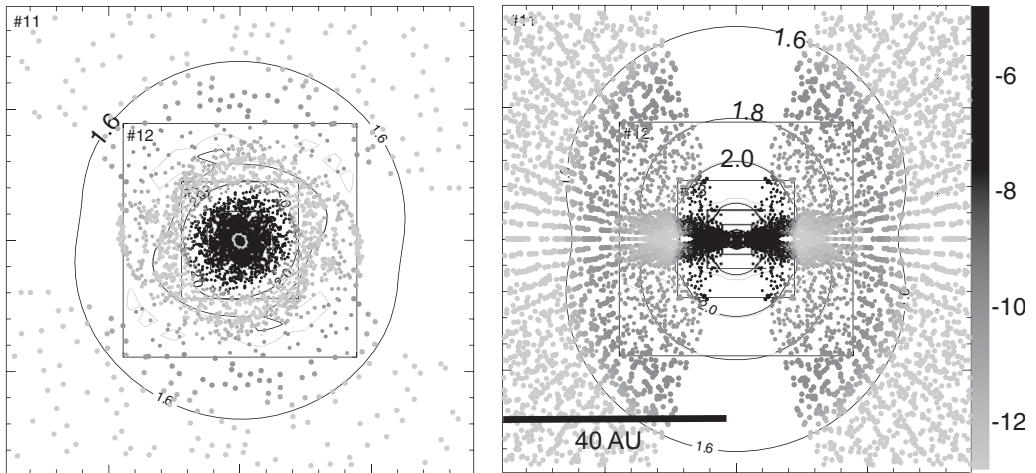
Figure 6. Spatial distribution of CH_3OH in the 3D first core model (gray dots). The line contours depict the temperature distribution in the $z = 0$ plane (left) and $y = 0$ plane (right).

4.2. *Molecular abundances*

In total we followed about 5000 fluid parcels and solved the gas-grain chemistry in each parcel. Figure 6 shows the abundances of gaseous CH_3OH in the x-z plane and the x-y plane. In the x-z plane, the CH_3OH distribution is almost spherical, simply following the temperature distribution. Our result indicates that CH_3OH can be a good tracer of the infalling envelope and the surface of the first core. In the x-y plane, on the other hand, the abundance decreases at the arms of the gravitational instability, where the density is slightly higher than the inter-arm region. In the zeroth approximation, the molecular abundances are determined by the gas-grain chemistry in the cold phase and sublimation at the temporal local temperature. Grain-surface reactions among heavy element molecules are limited, because the size of the warm ($T \sim$ several 10 K) envelope is small in the first core stage. Gas-phase reactions in the $T \geqslant 100$ K region is also limited by the short life time of the first core and the efficient mass accretion via gravitational instability.

5. Summary

We have investigated the molecular abundances and molecular D/H ratios in proto-stellar cores by calculating the detailed gas-grain chemical network model combined with the 1D and 3D radiation hydrodynamic models of star formation from cold dense cores to protostars. Our finding are as follows.

- While H_2CO and CH_3OH can be formed in molecular cloud conditions ($T \sim 10$ K), other large organic species such as CH_3CHO are formed mainly by the grain-surface reactions and gas-phase reactions at $T \sim$ several 10 K. In the infalling fluid parcels, such warm temperature lasts for $r_{warm}/v_{infall} \sim 10^4$ yr. Warm carbon chains are also formed from sublimated CH_4 at $T \geqslant 25$ K.

- While the spherical symmetry (1D model) is a good approximation in the envelope, a disk-like structures appears at $r \leqslant r_{cent}$. Duration of the warm temperature chemistry can be longer than mentioned above once the fluid parcels enter the disk region. The prolonged warm chemistry are favorable in producing some large organic species such as CH_3OCH_3 and $HCOOCH_3$, which are underestimated in our spherical model. It indicates that the envelope and the disk are characterized by different molecules in hot corinos.

• In both envelopes and disks, the large organic species and warm carbon chains are heavily deuterated. Although they are formed in the warm temperatures, their ingredients have high D/H ratios, which are set in the cold phase.

• In the first core, the molecular abundances are mostly determined by the local temperature and sublimation. For example, CH_3OH are abundant near the first core, and can be a good tracer of the infalling envelope and the surface of the first core.

References

Aikawa, Y., Herbst, E., Roberts, H., & Caselli, P. 2005, *ApJ*, 620, 330

Aikawa, Y., Wakelam, V., Garrod, R. T., & Herbst, E. 2008, *ApJ*, 674, 993

Cazaux, E., Tielens, A. G. G. M., Ceccarelli, C., Castets, A., Wakelam, V., Caux, E., Parise, B., & Teyssier, D. 2003, *ApJ*, 593, L51

Ceccarelli, C., Caselli, P., Herbst, E., Tielens, A. G. G. M., & Caux, E. 2007, *Protostars and Planets V*, ed. B. Reipurth, D. Jewitt, & K. Keil (Tucson: Univ. Arizona Press), 47

Chandler, C. J., Brogen, C. L., Shirley, Y. L., & Loinard, L. 2005, *ApJ*, 632, 371

Garrod, R. T. & Herbst, E. 2006, *A&A*, 457, 927

Harada, N., Herbst, E., & Wakelam, V. 2010, *ApJ*, 721, 1570

Hassel, G. E., Herbst, E., & Garrod, R. T. 2008, *ApJ*, 681, 1385

Klein, R. I., Inutsuka, S.-I., Padoan, P., & Tomisaka, K. 2007, *Protostars and Planets V*, ed. B. Reipurth, D. Jewitt, & K. Keil (Tucson: Univ. Arizona Press), 99

Kuan, Y.-J., *et al.*, 2004, *ApJ*, 616, L27

Larson, R. B. 1969, *MNRAS*, 145, 271

Machida, M. N., Matsumoto, T., Hanawa, T., & Tomisaka, K. 2005, *MNRAS*, 363, 382

Machida, M. N., Inutsuka, S., & Matsumoto, T. 2010, *ApJ*, 724, 1006

Masunaga, H., Miyama, S. M., & Inutsuka, S. 1998, *ApJ*, 495, 346

Masunaga, H. & Inutsuka, S. 2000, *ApJ*, 531, 350

Matsumoto, T. & Hanawa, T. 2003, *MNRAS*, 595, 913

Millar, T. J., Bennet, A., & Herbst, E. 1989, *ApJ*, 340, 906

Penston, M. V. 1969, *MNRAS*, 144, 425

Roberts, H., Herbst, E., & Millar, T. J. 2004, *ApJ*, 424, 905

Sakai, N., Sakai, T., Hitora, T., & Yamamoto, S., 2008, *ApJ*, 672, 371

Sakai, N., Sakai, T., Hitora, T., Burton, M., & Yamamoto, S., 2009, *ApJ*, 697, 769

Shu, F. 1977, *ApJ*, 214, 488

Tomida, K., Tomisaka, K., Matsumoto, T., Ohsuga, K., Machida, M. N., & Saigo, K., 2010, *ApJ*, 725, 239

Tomisaka, K. 2002, *ApJ*, 575, 306

Umebayashi, T., 1983, *PThPh*, 69, 480

Willacy K., Klahr H. H., Millar T. J., Henning T. H., 1998, *A&A*, 338, 995

Discussion

CABRIT: How well known are the rates of non-thermal ice desorption by UV and X-ray, and could this affect complex molecule abundances at later protostellar stages, where UV and X-ray from the central source become important?

AIKAWA: Effect of UV and X-ray would be restricted to the surface of the outflow cavity in the protostellar core (see Visser in this volume). Non-thermal desorptions are theoretically investigated by Léger, Jura & Omont (1985), and also recently examined in the laboratories. In our model UV radiation creates radicals on the grain surface, which then cause chemical desorption via reactions (i.e. a fraction of the reaction products are desorbed). We also include the non-thermal desorption by cosmic rays.

STERNBERG: Are your disks stable against fragmentation? Higher densities in clump fragments could reduce the chemical timescales.

AIKAWA: We chose the parameter (angular momentum of the initial core) so that the disk is stable against fragmentation. It would indeed be interesting to investigate the chemistry in fragmenting disks.

VITI: Just a comment that if you require complex molecules such as $HCOOCH_3$ to form on the grains at 10K, some experiments show you can make it via cosmic-ray irradiation e.g. see Poster by Occhiogrosso on the incorporation of these experiments into chemical models of pre-/proto-stellar cores.

AIKAWA: In order to include the experimental results on grain-surface formation of organic molecules to theoretical models, we need more than an apparent rate; we need to understand the elementary processes of the reaction quantitatively, e.g. as a function of ice mantle temperature and irradiation flux, etc. In our model, we have cosmic-ray induced UV radiation, which can produce radicals on grain surfaces. In order to make the complex molecules from these radicals, we need a mild heating to make them migrate (but not evaporate).

OSSENKOPF: How does turbulent chemical mixing, i.e. exchange of material between neighboring interacting cells change the results?

AIKAWA: In the envelope, mixing would not be important because of the geometry (spherical symmetry) and the fast infall velocities. In the forming disk, we think the effect of mixing is still very limited in our case, because of the short timescale of the object (i.e. the first core). The density is too high to activate the magneto-rotational instability, which is considered to be the main cause of turbulence in the class II disks. In our forming disk, radial mixing by the gravitational instability would be more important than the turbulent mixing; some fluid parcels are kicked by the arm and migrate to outer radii.