Composition of LHB Comets and Their Influence on the Early Earth Atmosphere Composition

C. Tornow • S. Kupper • M. Ilgner • E. Kührt • U. Motschmann

Abstract Two main processes were responsible for the composition of this atmosphere: chemical evolution of the volatile fraction of the accretion material forming the planet and the delivery of gases to the planetary surface by impactors during the late heavy bombardment (LHB). The amount and composition of the volatile fraction influences the outgassing of the Earth mantle during the last planetary formation period. A very weakened form of outgassing activity can still be observed today by examining the composition of volcanic gases. An enlightenment of the second process is based on the sparse records of the LHB impactors resulting from the composition of meteorites, observed cometary comas, and the impact material found on the Moon. However, for an assessment of the influence of the outgassing on the one hand and the LHB event on the other, one has to supplement the observations with numerical simulations of the formation of volatiles and their incorporation into the accretion material which is the precursors of planetary matter, comets and asteroids. These simulations are performed with a combined hydrodynamic-chemical model of the solar nebula (SN). We calculate the chemical composition of the gas and dust phase of the SN. From these data, we draw conclusions on the upper limits of the water content and the amount of carbon and nitrogen rich volatiles incorporated later into the accretion material. Knowing these limits we determine the portion of major gas compounds delivered during the LHB and compare it with the related quantities of the outgassed species.

Keywords impacts • solar nebula • hydrodynamic • chemistry

1 Fate of Volatiles During Planet Formation

Table 1 shows that the major gases (CO₂, H₂O, N₂, O₂) making 98-100% of the atmospheres of the three large rocky planets clearly vary in their concentrations. However, a completely different situation is observed for Mercury. Its atmosphere is incredibly thin, contains relatively large hydrogen and helium concentrations, and, in addition to oxygen, one finds a high fraction of sodium (29%). Both, the amount of hydrogen and helium and the existence of a large Na fraction indicate a strong interaction between the planet and the solar wind. This strong interaction is supported by the small distance to the Sun which causes a high radiation intensity (see Table 1) as well. Compared to the small radius and mass of the planet, it has an oversized iron core (note, its high density in Table 1) which could have been the result of a large mantle-stripping impact (Benz et al., 1988). Since the pressure and chemical composition of
Mercury's atmosphere differs so largely from the corresponding values of the other planets, we concentrate our study to Earth and partially Mars and Venus.

Table 1. Bulk, orbital and atmospheric parameter of the four rocky planets as observed today (http://nssdc.gsfc.nasa.gov/planetary/factsheet, Prinn & Fegley (1987), and). Note, that Mercury atmosphere additionally contains a large fraction of Na (29%). The normalisation values used in column 1 are: \( R_{\oplus} = 6.37 \times 10^6 \) m, \( M_{\oplus} = 5.97 \times 10^{24} \) kg, \( \rho_{\oplus} = 5.515 \) g/cm³, \( L_{\oplus} = 1.37 \times 10^3 \) W/m², 1 AU = 1.496×10¹¹ m, \( B_{\oplus} = 5 \times 10^{-5} \) T, and 1 bar = 10⁵ Pa.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mercury</th>
<th>Venus</th>
<th>Earth</th>
<th>Mars</th>
</tr>
</thead>
<tbody>
<tr>
<td>mean radius / ( R_{\oplus} )</td>
<td>0.383</td>
<td>0.950</td>
<td>1.00</td>
<td>0.532</td>
</tr>
<tr>
<td>mass / ( M_{\oplus} )</td>
<td>0.0553</td>
<td>0.815</td>
<td>1.00</td>
<td>0.107</td>
</tr>
<tr>
<td>mean density / ( \rho_{\oplus} )</td>
<td>0.984</td>
<td>0.951</td>
<td>1.00</td>
<td>0.713</td>
</tr>
<tr>
<td>solar irradiance / ( L_{\oplus} )</td>
<td>6.67</td>
<td>1.91</td>
<td>1.00</td>
<td>0.431</td>
</tr>
<tr>
<td>semi-major axis / AU</td>
<td>0.387</td>
<td>0.723</td>
<td>1.00</td>
<td>1.52</td>
</tr>
<tr>
<td>magnetic field / ( B_{\oplus} )</td>
<td>~10⁻²</td>
<td>&lt; 10⁻⁵</td>
<td>1.00</td>
<td>-</td>
</tr>
<tr>
<td>surface pressure / bar</td>
<td>10⁻¹⁵</td>
<td>92</td>
<td>1.014</td>
<td>6.36×10⁻³</td>
</tr>
<tr>
<td>atmospheric composition with respect to major gasses in %</td>
<td>CO₂ -</td>
<td>96.5</td>
<td>0.038</td>
<td>95.3</td>
</tr>
<tr>
<td></td>
<td>H₂O -</td>
<td>2×10⁻⁴</td>
<td>~1</td>
<td>3×10⁻⁴</td>
</tr>
<tr>
<td></td>
<td>N₂ -</td>
<td>3.5</td>
<td>78.08</td>
<td>2.7</td>
</tr>
<tr>
<td></td>
<td>O₂ 42</td>
<td>-</td>
<td>20.95</td>
<td>0.13</td>
</tr>
<tr>
<td></td>
<td>H₂ 22</td>
<td>10⁻³</td>
<td>5.5×10⁻⁵</td>
<td>-</td>
</tr>
<tr>
<td>atmospheric composition with respect to rare gasses in ppm</td>
<td>(^{4}\text{He} 6×10^4)</td>
<td>12</td>
<td>5.24</td>
<td>1.4</td>
</tr>
<tr>
<td></td>
<td>(^{20}\text{Ne} -)</td>
<td>7</td>
<td>18.2</td>
<td>2.5</td>
</tr>
<tr>
<td></td>
<td>(^{36}\text{Ar} -)</td>
<td>31</td>
<td>9.34×10⁴</td>
<td>1.6×10⁴</td>
</tr>
<tr>
<td></td>
<td>(^{84}\text{Kr} -)</td>
<td>0.025</td>
<td>1.14</td>
<td>0.3</td>
</tr>
<tr>
<td></td>
<td>(^{130}\text{Xe} -)</td>
<td>&lt; 0.009</td>
<td>0.09</td>
<td>0.08</td>
</tr>
</tbody>
</table>

1.1 Planet Formation

Two aspects influence the chemical composition of a planetary atmosphere, the formation process of the planet and the planetary evolution due to internal forces (e.g. magnetic fields, volcanism, plate motion, erosion, evolution of life) and external phenomenons (e.g. solar wind, impacts). The formation process needs to be considered since it has influenced the amount and composition of the volatile fraction of the accretion material. This fraction was produced by hydrides and oxides of N and C bearing molecules in the SN. Its amount and composition depend on the formation time of the planet and the distance to the protosun. The evolution effect is characterised on the one hand by relatively short and powerful events
(e.g. impacts or volcanism) and on the other hand by continuous processes with a low immediate influence (e.g. magnetic fields or solar wind).

The influence of Earth evolution on the fractional abundances of the major gases in the atmosphere is shown in Figure 1. Due to the sparse records not much is known about the Hadean eon (4.6-3.8×10^9 years) which also comprises planet formation. However, in order to understand where the carbon dioxide, water, and nitrogen content of the early atmosphere was coming from, one has to consider the scenario of inner planet formation in detail. It is based on core accretion and can be divided into four periods:

- pebble formation (> 1 mm) by dust coagulation and settlement into disk midplane with a ~ 10^4 y timescale,
- planetesimal formation (> 10^2 km) due to gravitational collapse of pebble clusters formed in various turbulence producing instability regions with a 10^3 - 10^4 y timescale,
- protoplanet formation (10^2-10^3 km) by gravitational cleaning of related feeding zones with a 10^5 - 10^6 y timescale and in two phases, which are
  - a runaway accretion phase with a relative growth rate given by dM/Mdt ~ M^{1/3}, and
  - an oligarchic accretion phase with a relative growth rate given by dM/Mdt ~ M^{-1/3}
- planet formation (10^4 km) by chaotic accretion due to giant impact events causing mergers of protoplanets (e.g. Moon forming impact) with a time-scale between 10^7 and 10^8 years.

Concerning the first two phases, it was shown by Johansen et al. (2007), Lyra et al. (2008), and Brauer et al. (2008) that the planetary embryos with a radius larger than 10^3 km could have been formed after a period of coagulation and settling. Planetesimal formation causes a mainly a physical modification of the accretion material. If one compares porosity values observed for cometary dust P_{CD} ~ 0.85 (Greenberg & Li, 1999) with porosities of the C-and D-type asteroids (0.5 - 0.6) (Trigo-Rodriguez & Blum, 2009) one realises the increased compactification due to collisions. This fits perfectly to observations of enstatite chondrites (Macke et al., 2009) coming from large solid bodies which are highly compactified (porosity ≤ 0.06). In addition to compactification protoplanet and planet formation leads to chemical modification resulting in an increase of insoluble organic matter and a decrease of the soluble fraction. This modification results in an increase of carbonaceous matter and a decrease of H and N containing molecules.

**Figure 1.** Concentration in percentage, C, shown for the major atmospheric gases of the Earth versus time in Gyr (1 Gyr = 10^9 years) whereby today is set to 0 Gyr (data except for NH_3 are from Kasting, 2004 and Kaltenegger et al., 2007). Note, that the time is logarithmically scaled and the concentrations of the reducing molecules CH_4 and NH_3 are given in 100% – C(CH_4) and 100% – C(NH_3), respectively.
In the simulations of O'Brien et al. (2006) a mixture of protoplanets with Mars-like masses and many large planetesimals is assumed to be the initial population of the accretion of rocky planets. This assumption agrees with the products of runaway and oligarchic accretion and describes the final, chaotic period of accretion. The chaotic period explains why the volatile concentration of the Earth does not agree with an equilibrium condensate formed at the pressure and temperature in the SN at 1 AU (Prinn & Fegley, 1987). In this period one has to take into account an outgassing of the planetary mantle of the three planets.

There is much evidence that water and CO₂ are typical substances outgassed from the mantle. According to Matsui (1993), Zahnle (1998) and references therein during the chaotic accretion period a magma ocean (depth: ~ 2000 km) with a steam atmosphere of ≥100 bar and a surface temperature of ~ 1500 K has been formed on Earth. In the course of 5×10⁷ years (Elkins-Tanton, 2008) the surface has cooled enough to allow the formation of a proto-ocean. According to model results (Kuramoto & Matsui, 1993, Elkins-Tanton, 2008) a local magma ocean could have been formed for Mars as well, but the ocean must have been more shallow in order to form a wet mantle and allow water outgassing. In contrast, due to the more intensive solar radiation on Venus (see Table 1) a hydrosphere was probably not formed on this planet (Abe, 1988).

1.2 Water

Now, we have to ask for the sources of water, carbon dioxide, and nitrogen which are contained in the early atmosphere (Figure 1). At first, there are indications that the planetesimals contained water gathered by physisorption and chemisorption (Stimpfl et al., 2006). The high adsorption energy of chemisorption found for forsterite ensures that water is held by the mineral surface at environmental temperatures of 700 K -1000 K. These values are typical for the inner region of the SN. Consequently water could have contained already in protoplanets formed in the inner SN. According to Morbidelli et al. (2000) during chaotic accretion a further reservoirs results from the outer asteroid belt. The parent bodies of carbonaceous chondrites and, if their number was large, main belt comets (Hsieh and David Jewitt, 2006) could have contributed to a large fraction of water. Observations have shown that D/H ratio of these bodies (~ 1.3×10⁻⁴; Kerridge, 1985) is comparable to \( D/H_{\text{SMOW}} = 1.56\times10^{-4} \), whereby SMOW stands for standard mean ocean water.

1.3 Carbon

In the inner region of the SN carbon is contained in the dust grains since main components are SiC compounds and refractive organic matter (e.g. kerogen-like substances). In addition large amounts of carbon is stored in polycyclic aromatic hydrocarbons (PAHs) which are nano-size particles collected by the larger dust grains during their settling to the midplane (Zubko et al., 2004). In the outer region of the SN, i.e., behind the snow line, carbon bearing molecules were incorporated in the ice mantle of dust grain or later as CH₄ clathrates in pebble clusters (Lunine & Stevenson, 1985).

1.4 Nitrogen

The sources of nitrogen are less known. It is very likely that the SN has contained N₂, but observations (Armitage et al., 2003; Sicilia-Aguilar et al., 2007) suggest that the gas of the nebula was blown away after less than 10 Ma, depending on the frequency range and intensity of the stellar UV radiation in the environment of the SN. A protoplanet, which can be formed in 10⁵ to 10⁶ years, has gathered enough
mass to keep the SN gas as a primary atmosphere. According to the calculations of Genda & Abe (2003) in which the Moon forming impact was considered, it is likely that the Earth was able to keep at least 70% of its primary atmosphere. In addition, an N-bearing substance (Si$_3$N$_4$) was found in ordinary chondrites (Lee et al., 1995). Clément et al. (2005) have detected features in the infrared spectrum of carbon stars which coincide well with the main features of laboratory Si$_3$N$_4$ spectra. Consequently, these nitrides are of interstellar origin. Further, N$_2$ could have been added to the Earth atmosphere during the LHB. We will consider this possibility in more detail in section 3.

2 Atmospheric Composition After Earth Formation

Due to the formation of life on Earth the current atmospheric composition differs clearly from the composition directly after the formation of the planet. In order to understand the influence of the LHB comets on the early Earth atmosphere we need a solidified assumption concerning the composition directly after planet formation as a starting point. According to the reflections in the previous section the atmosphere of the rocky planets contained as major gases CO$_2$ and N$_2$. Table 1 shows that for Mars and Venus the carbon dioxide fraction is large (95 - 96%) while the nitrogen fraction is relatively small (3 - 4%). The water fraction disappeared on both planets. Mars has lost its water due to the disappearance of its magnetic field. Thus, in addition to thermal ejection the solar wind could have stripped away its atmosphere. The surface cooling and pressure decreasing have given a situation in which water ice sublimated and due to the solar UV radiation the molecule dissociated. H$_2$ has left the planet and O has oxidised minerals on the planetary surface. However, a part of the water ice has survived and is probably buried under the dust. Concerning Venus, it was already mentioned that no hydrosphere was formed due to the high temperature. Similar to Mars, Venus has presumably no magnetic field and the water vapour molecules have been dissociated by the strong solar UV radiation. In contrast to Mars, Venus has lost large amounts of hydrogen and oxygen by nonthermal processes such as ion pick-up (Lammer et al., 2006). If one assumes no large differences in the chemical composition of the accretion material and compares the current D/H ratios (Lammer et al., 2008) of Earth ($1.5 \times 10^{-4}$), Mars ($8.1 \times 10^{-4}$), and Venus ($2 \times 10^{-7}$) it follows that the loss of H$_2$O molecules on Earth was least important.

If one constructs an atmospheric composition of the early Earth we take a CO$_2$/N$_2$ ratio as observed for today for Mars and Venus. As a result, 78% N$_2$ of the Earth atmosphere today correspond to 3-5% N$_2$ for the early case. The resulting early pressure varies between 15-26 bar produced by a CO$_2$ atmosphere. Is the related amount of carbon available on Earth? Table 2 presents the current mixing ratios for the most important volatiles at the time directly after planet formation. We see, that on Venus nearly the complete amount of carbon dioxide, nitrogen, and water are contained in the atmosphere. On Mars and Earth this is true for nitrogen only. A large amount of CO$_2$ on Earth and Mars is in a condensed phase. On Mars we have CO$_2$ ice and on Earth the equilibrium reaction

$$\text{Mg}_2\text{SiO}_4 + 4\text{CO}_2 + 4\text{H}_2\text{O} \rightleftharpoons 2\text{Mg}^{2+} + 4\text{HCO}_3^- + \text{H}_4\text{SiO}_4$$

which describes weathering via hydrolysis and carbon dioxide dissolution in water, controls the amount of carbon in the condensed and gaseous phase. The mineral Mg$_2$SiO$_4$ symbolises olivine, i.e. forsterite, HCO$_3^-$ denotes a bicarbonate ion, and H$_4$SiO$_4$ is silicic acid. Other, more complex, weathering reactions are possible as well, for instance with feldspar (KAlSi$_3$O$_8$). According to Pidwirny (2006) there are $7-10 \times 10^{22}$ g carbon dioxide available on Earth and the resulting pressure ~ 20 bar. From Table 2 one realizes a much larger amount of water (Lide, 2001) which is given by $1.4 \times 10^{24}$ g which would produce
a pressure of ~ 290 bar. This is close to the upper limit of the calculations of Zahnle, 1998. However an outflow during the phase of magma ocean and steam atmosphere as well as a large water component stored in the planetary mantle cannot be excluded. As the surface has cooled down sufficiently a shallow oceans formed about 4.4×10⁹ years ago (compare with Wilde et al., 2001). The CO₂ and water amounts fit well to the data given in Table 2.

Table 2. Global mass fraction of volatile substances stored in the bulk planet and in the atmosphere today. The masses of the planets follow from Table 1. The data are given in Goody & Walker (1972).

<table>
<thead>
<tr>
<th>Substance</th>
<th>Site</th>
<th>Venus</th>
<th>Earth</th>
<th>Mars</th>
</tr>
</thead>
<tbody>
<tr>
<td>carbon dioxide</td>
<td>bulk planet</td>
<td>1.2×10⁻⁴</td>
<td>1.8×10⁻⁵</td>
<td>3.1×10⁻⁶</td>
</tr>
<tr>
<td></td>
<td>atmosphere</td>
<td>8.7×10⁻⁵</td>
<td>4.4×10⁻¹⁰</td>
<td>3.0×10⁻⁸</td>
</tr>
<tr>
<td>nitrogen</td>
<td>bulk planet</td>
<td>1.5×10⁻⁶</td>
<td>1.2×10⁻⁶</td>
<td>2.0×10⁻¹⁰</td>
</tr>
<tr>
<td></td>
<td>atmosphere</td>
<td>1.1×10⁻⁶</td>
<td>5.8×10⁻⁷</td>
<td>1.7×10⁻¹⁰</td>
</tr>
<tr>
<td>water</td>
<td>bulk planet</td>
<td>2.0×10⁻⁹</td>
<td>2.3×10⁻⁴</td>
<td>3.9×10⁻⁶</td>
</tr>
<tr>
<td></td>
<td>atmosphere</td>
<td>1.6×10⁻⁹</td>
<td>2.5×10⁻⁹</td>
<td>2.2×10⁻¹²</td>
</tr>
</tbody>
</table>

Finally we have to consider the different types of accretion material. Based on equilibrium calculations and for an atmospheric state derived from an impact atmosphere (Abe & Matsui, 1987) a gas composition is determined by Schaefer & Fegley (2010). The obtained data important to evaluate our assumed atmospheric composition are shown in Table 3 for four different chondrite types (CI, CM are carbonaceous chondrites with very pristine material, L is an ordinary chondrite with a low amount of oxidized iron, and EH is an enstatite chondrite with a high amount of iron and non-oxidized iron). The most pristine material is fond for carbonaceous chondrites of the type CI while the CM chondrites experienced an extensive aqueous alteration. L and EH chondrites contain reducing material and CI and CM produce a neutral composition. For our evaluation we use the CO₂/N₂ ratio, which is given for an early atmosphere by a value ranging between 15-32. A composition of CM and L chondrites produces nearly the same range: 15-33. The same order of agreement was not reached for the ratio H₂O/CO₂ which gives ~ 15 for the early atmosphere and 3-5 for CM and L chondrites. We have not used the EH values since in this case the agreement to early Earth rations becomes worse.

Table 3. Gas compositions of impact generated atmospheres from chondritic planetesimals at 1500 K and 100 bars.

<table>
<thead>
<tr>
<th>substance</th>
<th>CI</th>
<th>CM</th>
<th>L</th>
<th>EL</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂O</td>
<td>69.47</td>
<td>73.38</td>
<td>17.43</td>
<td>5.71</td>
</tr>
<tr>
<td>CO₂</td>
<td>19.39</td>
<td>18.66</td>
<td>5.08</td>
<td>9.91</td>
</tr>
<tr>
<td>N₂</td>
<td>0.82</td>
<td>0.57</td>
<td>0.33</td>
<td>1.85</td>
</tr>
<tr>
<td>H₂</td>
<td>4.36</td>
<td>2.72</td>
<td>42.99</td>
<td>14.87</td>
</tr>
<tr>
<td>CO</td>
<td>3.15</td>
<td>1.79</td>
<td>32.51</td>
<td>67.00</td>
</tr>
<tr>
<td>H₂S</td>
<td>2.47</td>
<td>2.32</td>
<td>0.61</td>
<td>0.18</td>
</tr>
</tbody>
</table>

Now we have determined an early chemical composition and found that the early atmosphere was mainly neutral. However for the formation of life one needs a more reducing environment. Since SN chemistry is hydrogen chemistry the LHB comets could have a more reducing influence. Thus, the retention of the primary atmosphere and the delivery of volatile molecules by LHB comets will increase
the reducing character of the Earth atmosphere and improve the chances of life formation. Observations from Schopf (1993) and Brazier et al. (2002) have shown that life on the Earth probably formed somewhere around $3.5 \times 10^9$ years or perhaps even earlier (Mojzsis et al., 1996; van Zuilen et al., 2002; Cate & Mojzsis, 2006). Unfortunately, there is not much evidence left from this time to describe the geological state of the planet and the thermodynamic one of its atmosphere.

3 Calculation of Nitrogen Bearing Molecules in SN

We simulate chemical processes in each of the three evolution periods considered in our solar nebula model. We discriminate between

- a quasi-static prestellar core,
- a collapsing protostellar core, and
- an evolving turbulent disk.

Our purpose is to identify chemical species that were incorporated into comets in a sufficiently large number. Especially, we have made great efforts in order to derive a realistic and compact hydrodynamic models to describe the evolutionary periods of the solar nebula.

Table 4. The three phases of the multi-zone solar nebula model.

<table>
<thead>
<tr>
<th>Dark cloud with quasi-static prestellar cores</th>
<th>Collapsing protostellar core</th>
<th>Evolving turbulent disk with protosun</th>
</tr>
</thead>
</table>

3.1 Quasi-static Prestellar Core

The quasi-static evolution of a prestellar core is modelled with a linear time dependency of the temperature and density. Systematic flow processes are not considered. The negligence of flows and unsteady evolution events such as shock waves or cloud collisions is justified since the temperature and density of the cloud core change over the large time interval of nearly 15 million years. The relative abundances of species $i$ in the gas and ice phase $x_i$ and $x_i^*$, respectively, are calculated from a set of kinetic equations. The rates for the chemical reactions are computed from data of Woodall et al. (2007) and Aikawa et al. (1997).

Table 5 contains the initial abundances. We have restricted our set of species to compounds having no more than seven atoms. From the calculated abundance evolution we obtain the time dependence of the ratios shown in Figure 2. One recognises an increasing amount of non-polar ice and
bounded heavy isotopes in the course of the prestellar core evolution. A large $\text{H}_2$ to $\text{H}$ ratio seems to be advantageous for the formation of $\text{CO}_2$ relative to $\text{H}_2\text{O}$.

Table 5. Initial abundances relative to hydrogen abundance.

<table>
<thead>
<tr>
<th></th>
<th>H</th>
<th>H$_2$</th>
<th>D</th>
<th>He</th>
<th>O</th>
<th>C$^+$</th>
<th>N</th>
<th>Si</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.9</td>
<td>0.1</td>
<td>1.5$x10^{-5}$</td>
<td>0.14</td>
<td>1.8$x10^{-4}$</td>
<td>7.3$x10^{-5}$</td>
<td>2.1$x10^{-5}$</td>
<td>6.0$x10^{-11}$</td>
</tr>
</tbody>
</table>

Figure 2. Time dependency of the nitrogen isotope ratio in the gas phase (note the factor of 50 to present all curves in the same figure), the D/H ratios in the ice phase and the $\text{CO}_2$/H$_2$O ratio for the polar to non-polar ice fraction calculated for the slowly evolving quasi-stationary prestellar core.

3.2 Collapsing Protostellar Core

The gravitational collapse of a cloud core causes the central density to increase over more than 15-16 orders of magnitudes. At the end of this process a stellar core, the T Tauri star, and a young disk have formed in the centre of the solar nebula. Therefore, a numeric simulation of this type of collapse is a complex task.

We have derived an analytical solution to solve the continuity, momentum and Poisson equation for a collapsing cloud core in four radial zones using spherical symmetry. According to Saigo et al. (2008) the spherical symmetry has no serious drawbacks as long as the rotation rate is low $10^{-15}$ s$^{-1}$. The mathematics of this solution will be described in a different publication. In Figure 3 we present the calculated radial density, mass, velocity, and temperature profiles at different times. In order to include the influence of the formed protostellar disk we have coupled our collapse solution to the disk model derived by Stahler et al. (1994).

The values of the four radial profiles in Figure 3 are given for an Eulerian grid. However, the computation of the chemical abundance evolution of the gas and ice phase following from the continuity equation of each species can be simplified if one uses a transformation to a Lagrangian grid defined by the initial positions of the gas-ice parcels at the beginning of the collapse. The resulting total time dependencies of the density and temperature are calculated for an inner gas parcel moving from 2.5 to 1.3 AU. In this case the temperatures are high enough to guarantee the loss of the ice phase due to the
evaporation of the icy grain mantles. In order to study the temporal progress of depletion of the ice phase species we have computed the ratio of the current to the initial abundance for selected compounds. The obtained values are presented in Figure 4.

**Figure 3.** Radial profiles of density, mass, mass flow, and temperature for selected time points calculated with our analytical multi-zone model of the solar nebula. The vertical dotted lines in the left plots show the distribution of the zones at the beginning (upper plot) and at the end of the collapse period (lower plot).

**Figure 4.** Time dependency of the ratio of the current to the initial abundance for CO, H$_2$O, and NH$_3$ calculated for the period of the collapsing protostellar core.
3.3 Evolving Turbulent Disk

The disk model of Stahler et al. (1994), is valid for a young disk only. In order to study the chemical evolution of the gas and ice species in a mature disk we have used the non-stationary model of Davis (2003). This model describes the disk cooling and depletion in the course of its evolution. Due to the gas flow we have to switch to the Lagrangian grid again in order to compute the abundance values. The necessary initial data follow from the final abundance results calculated for the collapse period. In contrast to our collapse model the Davis model is based on axial symmetry. In order to keep a simple radial dependency without angular variations, the relative abundances are derived with respect to the column density. For time intervals much larger than $10^7$ the corresponding number density would be less than 0.01 cm$^{-3}$, i.e. a gas disk is not existent anymore. Therefore, at most 10 million years are of physical interest only. Figure 5 shows the time behaviour of the same ice ratios as seen in Figure 2. However, one recognizes clear differences although in both cases the ice phase abundancies are growing with respect of their initial values. For the evolving disk, there is a superposition of the time dynamics of the disk parameter itself and the time dynamics of the chemical processes. Thus, the shapes of the disk related abundance ratios versus time are less monotonic than the same curves of the prestellar core. Further, disk density of the considered gas parcel decreases whereas core density increases slowly.

Figure 5. Time dependency of the D/H ratios in the ice phase and the CO$_2$-H$_2$O molecular ratio for the polar to non-polar ice fraction calculated for the evolving disk.

4 Conclusion and Outlook

We have motivated the assumption that the ratio of CO$_2$/N$_2$ was nearly similar (i.e. ~ 15) for the atmospheres of Earth, Mars, and Venus directly after planet formation. In order to calculate the primarily reducing contribution of LHB comets to the Earth atmosphere we have combined a hydrodynamical model of the SN with a kinetic model to simulate the chemical evolution. Especially we have developed an analytical solution for the collapse period that gives the chance to simulate this process very efficiently. Both models, the hydrodynamic and the chemical, were thoroughly tested to guarantee the consistency of merging the evolution periods of the solar nebula using the transition from an Eulerian to a Lagrangian grid. However, the transition from the spherically collapsing cloud core to
the disk is complicated and further research needs to be done for the transition between the different temperature models.

From chemical calculations a distinct difference between disk and prestellar core chemistry becomes conspicuously. It is related to the higher dynamics in the disk on the one hand and to its complex initial chemical state on the other. The effects of both phenomenons are entangled and further research needs to be done to investigate their influence independently. Figure 6 allows to estimate the amount of nitrogen bearing molecules. According to Gomes et al. (2005) nearly $10^{22}$ g of material from LHB comets have reached the Earth surface. The ice formed by soluble matter amounts 25 - 33%. Thus one gets $2.5 \times 10^{21}$ g and the corresponding N amount is not more than 1 - 5 % giving $\geq 2.5 \times 10^{19}$ g (see indications in Figure 6). If we compare this contribution with the current mass of the biosphere ($10^{19}$ g). Consequently, the LHB comets might have delivered an amount of reducing and soluble material important for life formation in a otherwise neutral atmosphere. In a next study we will calculate the amount of reducing gasses from the SN retained by the Earth during its formation process.

![Figure 6](image)

**Figure 6.** Abundance ratios versus time in years. The evolution of the three major nitrogen bearing molecules in the ice phase of the solar nebula is illustrated, whereby "CN" stands for the abundance of HCN + HC$_3$N.

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