Chapter 6b – Big Bang Nucleosynthesis

Last Update: 25 June 2006

1. Introduction

In Chapter 6 we saw how the ratio of the numbers of protons to neutrons was established in the first few minutes after the big bang, namely 87.5%:12.5%. The neutrons, unstable when free, find sanctuary in stable nuclei, almost entirely helium-4. In that Chapter we avoided the complex issue of the many interacting nuclear reactions, and how these lead to the final abundances of the other light nuclei: deuterium, helium-3 and lithium-7. Since these nuclei are stable it is not immediately obvious why they turn out to be only trace elements. In this Chapter we return to this topic and derive their abundances. We shall consider elements up to helium only. More complete treatments show that lithium-7 is also produced. However, its abundance is about four orders of magnitude less than that of helium-3 and deuterium, which in turn are about four orders of magnitude less abundant than helium-4.

Before turning attention to the deuterium and helium-3 abundances, we shall briefly revisit the issue of the time (temperature) at which deuterons become stable against photodisintegration. This marks the start of the period of Big Bang nucleosynthesis. In Chapter 6 we made an approximate assessment of deuteron stability against photodisintegration based on a simple count of the number of photons with sufficient energy (>2.224 MeV). In the next Section we shall treat this problem with a more powerful analytical tool which allows the density of deuterons to be determined at each time (temperature) if fusion beyond deuterium did not occur. The greater detail provided by this analysis regarding the onset of deuteron stability is helpful in orienting our thinking in subsequent Sections dealing with the true deuteron and helium-3 abundances.

The period of Big Bang nucleosynthesis will be found to last only a few minutes. There are two reasons for this. The first is that temperature and density are reducing rapidly in the expanding universe. Since nuclear fusion reactions are extremely sensitive to temperature, this leads to rapidly reducing reaction rates. In addition, reaction freeze-out by universal expansion, as discussed previously in Chapter 6, turns out to be important in establishing the termination of some reactions, and hence the final abundances. Most of the fusion activity occurs in the period 100 to 200 seconds. Reactions have virtually ceased by about 500 seconds.

2. Deuteron Density Versus Time (If No Further Fusion Reactions Occurred)

In this Section we calculate the deuteron density against time (temperature). The calculation will be based on the fiction that no subsequent nuclear reactions take place beyond the formation of deuterium. Thus, the derived deuteron density is a monotonically increasing function. In reality, subsequent reactions deplete the deuteron density – very markedly in fact, since the residual deuteron density is very low. Consequently, once a significant density of deuterons has formed, this derivation will not be correct. Nevertheless, we expect the approximate time-frame over which the (mythical) deuteron abundance builds from nothing to its maximum level will correspond roughly to the period of nucleosynthesis. This is the purpose of making this preliminary assessment.

The method employed is explained in detail in Chapter 8 (where the application is the formation of neutral atoms, due to capture of electrons by nuclei). Briefly, equilibrium concentrations of the reacting species are determined by minimising the Helmholtz free energy. This is shown to be equivalent to minimising the partition function with respect to the particle density. The method applies when the photons may be assumed to be a constant temperature heat bath. This applies here since the far greater energy density of the photon field means that its temperature is negligibly affected by the neutron/proton capture to form deuterons. Following Chapter 8, Equ.(37), the partition functions for the neutrons, protons and deuterons, treated as separate sub-systems are,

$$Z_n = \frac{\sqrt{\pi}}{4} \cdot \frac{V}{\pi^2 \hbar^3} \left(2M_n kT\right)^{3/2} e^{-M_n c^2 / kT} \tag{1}$$

$$Z_p = \frac{\sqrt{\pi}}{4} \cdot \frac{V}{\pi^2 \hbar^3} \left(2M_p kT\right)^{3/2} e^{-M_{pn} c^2 / kT} \tag{2}$$

$$Z_D = \frac{3}{2} \cdot \frac{\sqrt{\pi}}{4} \cdot \frac{V}{\pi^2 \hbar^3} \left(2M_D kT\right)^{3/2} e^{-M_D c^2 / kT} \tag{3}$$

where the factor of 3/2 in the deuteron expression, (3), arises because the deuteron has 3 spin states (i.e. it is spin 1) rather than 2.

V is an arbitrary volume within which the initial numbers of protons and neutrons are,

$$N_p^0 = 0.875 V \rho_b \qquad \text{and} \qquad N_n^0 = 0.125 V \rho_b \tag{4}$$

where the baryon density is given by,

$$\rho_b = \rho_\gamma / \xi \qquad \xi = 1.9 \text{ x } 10^9 \qquad \rho_\gamma = 0.2436 \left(\frac{kT}{\hbar c} \right)^3 \tag{5}$$

Thus, in Equ.(4) we have assumed, for simplicity, the result of Chapter 6 for the ratio of protons to neutrons. The problem thus has just one degree of freedom: the density of deuterons at each time, ρ_D, or equivalently, the number of deuterons in our arbitrary volume, $N_D = V\rho_D$. The densities of the remaining free protons and free neutrons are thus,

$$\rho_p = \rho_p^0 - \rho_D \qquad \text{or} \qquad N_p = N_p^0 - N_D \tag{6}$$

$$\rho_n = \rho_n^0 - \rho_D \qquad \text{or} \qquad N_n = N_n^0 - N_D \tag{7}$$

Hence, as discussed in Chapter 8, the partition function for the combined system comprising of the neutrons, protons and deuterons is,

$$Z = \frac{Z_n^{N_n^0 - N_D} Z_p^{N_p^0 - N_D} Z_D^{N_D}}{(N_n^0 - N_D)!(N_p^0 - N_D)!N_D!} \tag{8}$$

and minimising this by setting the derivative of Z with respect to N_D to zero results in,

$$\frac{(N_n^0 - N_D)(N_p^0 - N_D)}{N_D} = \frac{Z_n Z_p}{Z_D} \tag{9}$$

The particle densities are conveniently normalised by the total baryon density at each instant, by defining,

$$f_D = \rho_D / \rho_b \quad \text{and} \quad f_n^0 = \rho_n^0 / \rho_b = 0.125 \quad \text{and} \quad f_p^0 = \rho_p^0 / \rho_b = 0.875 \tag{10}$$

In terms of which, and using Equs.(1, 2, 3), Equ.(9) becomes,

$$\frac{\left(f_n^0 - f_D\right)\left(f_p^0 - f_D\right)}{f_D} = \frac{4}{3} \cdot \left(\frac{M_n M_p kT}{2\pi M_D \hbar^2}\right)^{3/2} \frac{1}{\rho_b} \cdot e^{-\Delta Mc^2 / kT} \tag{11}$$

where, $\Delta M = M_n + M_p - M_D$ (i.e. $\Delta Mc^2 = 2.2245\,\text{MeV}$) (12)

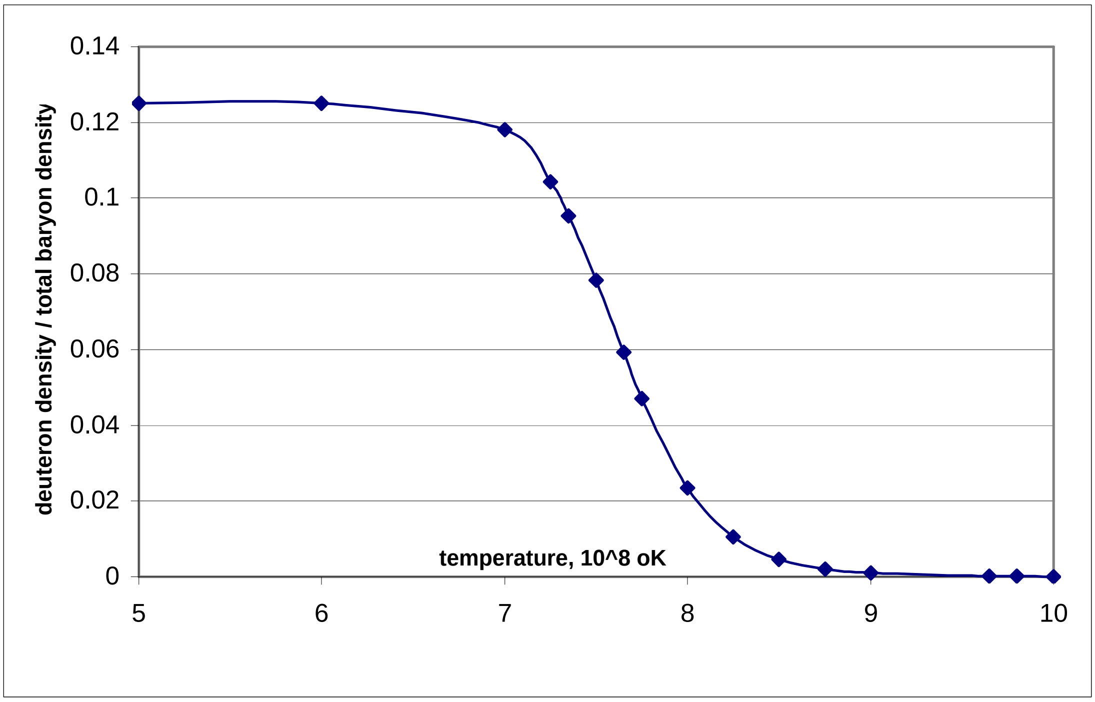
Thus, Equ.(11) determines the (normalised) deuteron density f_D at any required temperature. Substituting the total baryon density from Equ.(5) gives,

$$\begin{aligned} \frac{\left(f_n^0 - f_D\right)\left(f_p^0 - f_D\right)}{f_D} &= 0.348\xi \left(\frac{M_n M_p c^2}{M_D kT}\right)^{3/2} e^{-\Delta Mc^2 / kT} \\ &= 6.60\text{x}10^8 \left(\frac{470.016\text{MeV}}{kT}\right)^{3/2} e^{-2.2245\text{MeV}/kT} \end{aligned} \tag{13}$$

Hence we find the results for the deuteron density as follows,

t (sec)	**T (10^8 °K)**	**f_D**	**t (sec)**	**T (10^8 °K)**	**f_D**
93	10.6	0.0000166	163	8.0	0.0234
96	10.4	0.0000257	174	7.75	0.0471
100	10.2	0.0000406	178	7.65	0.0593
104	10.0	0.0000650	185	7.50	0.0783
109	9.8	0.000104	193	7.35	0.0953
112	9.65	0.000159	198	7.25	0.1043
129	9.0	0.000973	213	7.0	0.118
136	8.75	0.00209	290	6.0	0.12498
144	8.5	0.00465	417	5.0	0.125 = f_n^0
153	8.25	0.01054			

At time 290 seconds the deuteron number density would be within ~0.02% of the limiting value, i.e. the available neutron density, f_n^0 - IF no deuteron consuming reactions took place. This, of course, is fictional. At the time estimated for deuteron stability in Chapter 6, i.e. 136 seconds, we see that only about 2% of the deuterons have yet formed. About 50% of the deuterons have formed by 180 seconds (3 mins), at a temperature of 7.6 x 10^8 ^{o}K. The above results are plotted graphically below, noting that time increases to the left…



The above estimates of deuteron densities, being based upon the assumption of thermodynamic equilibrium, are valid only if the reaction rate between n and p to form D is sufficiently fast. If not, thermodynamic equilibrium would not have time to be established. It is easy to check that the reactions are indeed sufficiently fast. However, we will not dwell upon this since the calculation of this Section is purely hypothetical in any case. The subsequent reactions which consume deuterium are even faster, and this leads to maximum deuteron densities which are orders of magnitude smaller than implied above.

3. The Subsequent Nuclear Reactions and Their Rates

The preceding Section has considered the thermodynamic equilibrium between the fusion and photodisintegration reactions,

[1b] $\quad {}^1_1p + {}^1_0n \rightarrow {}^2_1D + \gamma$ $\qquad$ Exothermic: $0 \rightarrow 2.2245$ MeV

[γ] $\quad {}^2_1D + \gamma \rightarrow {}^1_1p + {}^1_0n$ $\qquad$ Endothermic: $2.2245 \rightarrow 0$ MeV

Once a non-zero deuteron density has been established, however, other fusion reactions will also take place. In a notation that will be used again in Chapter 13 these reactions are;

		Change in Binding Energy (MeV)
[2]	${}^1_1p + {}^2_1D \rightarrow {}^3_2He + \gamma$	$2.2245 \rightarrow 7.718$
[3]	${}^3_2He + {}^3_2He \rightarrow {}^4_2He + 2{}^1_1p$	$2 \times 7.718 \rightarrow 28.296$
[a]	${}^2_1D + {}^2_1D \rightarrow {}^4_2He + \gamma$	$2 \times 2.2245 \rightarrow 28.296$
[b]	${}^2_1D + {}^2_1D \rightarrow {}^3_1H + {}^1_1p$	$2 \times 2.2245 \rightarrow 8.482$
[c]	${}^2_1D + {}^2_1D \rightarrow {}^3_2He + {}^1_0n$	$2 \times 2.2245 \rightarrow 7.718$
[d]	${}^3_1H + {}^2_1D \rightarrow {}^4_2He + {}^1_0n$	$8.482 + 2.2245 \rightarrow 28.296$
[e]	${}^3_2He + {}^1_0n \rightarrow {}^3_1H + {}^1_1p$	$7.718 \rightarrow 8.482$
[f]	${}^1_0n + {}^2_1D \rightarrow {}^3_1H + \gamma$	$2.2245 \rightarrow 8.482$
[g]	${}^3_1H + {}^1_1p \rightarrow {}^4_2He + \gamma$	$8.482 \rightarrow 28.296$
[h]	${}^3_2He + {}^1_0n \rightarrow {}^4_2He + \gamma$	$7.718 \rightarrow 28.296$
[i]	${}^3_2He + {}^2_1D \rightarrow {}^4_2He + {}^1_1p$	$7.718 + 2.2245 \rightarrow 28.296$
[j]	${}^3_2He + {}^3_1H \rightarrow {}^4_2He + {}^2_1D$	$7.718 + 8.482 \rightarrow 28.296 + 2.245$
[k]	${}^3_2He + {}^3_1H \rightarrow {}^4_2He + {}^1_0n + {}^1_1p$	$7.718 + 8.482 \rightarrow 28.296$

These reactions have all been written with the forward direction being exothermic. The figures on the right indicate the binding energies on the two sides (in MeV). The difference in the binding energies on the two sides is the gain in kinetic energy of the products (carried off predominantly by the lighter particle). In principle, all these reactions are reversible. However, the endothermic energy requirements for the reverse reactions are large in all cases (except possibly [e]) compared with the prevailing thermal energies, even when account is taken of the numerical superiority of the photons. Hence, we do not expect the reverse reactions to play a major role except in the case of photodisintegration, reaction [γ].

The rates of some of the forward reactions, in s^{-1} per mole/cm^3, are:-

T (^oK)	**[1b]**	**[2]**	**[3]**	**[a]**	**[b]**	**[g]**
10^7	4.37×10^4	-	1.2×10^{-13}	1.4×10^{-6}	11.9	-
1.4×10^7	4.37×10^4	0.0036(1)	3.3×10^{-12}	4.0×10^{-6}		0.1
3×10^7	4.37×10^4	0.21	2.1×10^{-6}	2.8×10^{-4}	2,500	1.1
5×10^7	4.37×10^4	1.10	7.1×10^{-4}	1.7×10^{-3}	15,400	6.0
10^8	4.37×10^4	7.0	0.417	0.0116	110,000	39.0
3×10^8	4.37×10^4	65.0	623.0	0.0914	1.06×10^6	370.0
5×10^8	4.37×10^4	150.0	7750.0	0.176	2.51×10^6	890.0
10^9	4.37×10^4	390.0	134,000	0.359	7.78×10^6	2,600
1.5×10^9	4.37×10^4	630.0	605,000	0.530	1.53×10^7	4,700
2×10^9	4.37×10^4	870.0	1.71×10^6	0.715	2.49×10^7	7,100

(1)*Extrapolated (uncertain)* *(from Hoffman et al)*

The rates of the remaining forward reactions, in s^{-1} per mole/cm^3, are:-

T (^oK)	**[c]**	**[d]**	**[e]**	**[f]**	**[h]**	**[i]**	**[j]**	**[k]**
3×10^8	1.21×10^6	3.43×10^8	0	69	4.0	4.76×10^6	9.82×10^4	1.41×10^5
4×10^8						1.23×10^7	2.24×10^5	3.23×10^5
5×10^8	3.01×10^6	4.87×10^8	0	69	4.0	2.22×10^7	3.94×10^5	5.71×10^5
7×10^8						4.53×10^7	8.27×10^5	1.21×10^6
10^9	9.75×10^6	5.17×10^8	0	69	4.0	7.81×10^7	1.58×10^6	2.32×10^6
1.5×10^9	1.93×10^7	4.70×10^8	0	69	4.0	1.13×10^8	2.79×10^6	4.15×10^6

(from Hoffman et al)

Closed-form expressions for the reaction rates which allow interpolations for temperatures between 5×10^8 and 10^9 ^oK, are:-

Rate [2] = $1.529 \times 10^{-10} T^{1.3785}$
Rate [3] = $1.3185 \times 10^{-32} T^{4.1119}$
Rate [a] = $1.99 \times 10^{-10} T^{1.0284}$
Rate [b] = $1.593 \times 10^{-8} T^{1.6321}$
Rate [c] = $5.35 \times 10^{-9} T^{1.6956}$
Rate [d] = $6.11 \times 10^8 - 0.094T$
Rate [g] = $3.128 \times 10^{-11} T^{1.5466}$
Rate [i] = $1.408 \times 10^{-6} T^{1.5271}$
Rate [j] = $7.301 \times 10^{-11} T^{1.8150}$
Rate [k] = $8.712 \times 10^{-11} T^{1.8250}$
(the remaining reactions have constant rates).

The one reaction whose rate we have not given above is that of photodisintegration, reaction [γ]. A closed-form expression for the rate of this reaction at any temperature T is derived in Appendix A6.

4. Formulation of the Problem

We use a notation in which [r] stands for the rate of reaction 'r', and ρ_X is the number density of nucleus X. For convenience we collect together the contributions to the rates of production and consumption for each nuclear species. Thus, if $\uparrow$ and $\downarrow$ represent production and consumption rates respectively, we have,

$$\dot{\rho}_{D\uparrow} = \rho_p \rho_n [1b] + \rho_{He3} \rho_t [j] \quad (14)$$

$$\dot{\rho}_{D\downarrow} = \rho_p \rho_D [2] + 2\rho_D^2 ([b]+[c]) + \rho_t \rho_D [d] + \rho_n \rho_D [f] + \rho_{He3} \rho_D [i] + \rho_D^2 [a] + \rho_D [\gamma] \quad (15)$$

$$\dot{\rho}_{t\uparrow} = \rho_D^2 [b] + \rho_n \rho_D [f] \quad (16)$$

$$\dot{\rho}_{t\downarrow} = \rho_t \rho_D [d] + \rho_t \rho_p [g] + \rho_{He3} \rho_t ([j]+[k]) \quad (17)$$

$$\dot{\rho}_{He3\uparrow} = \rho_p \rho_D [2] + \rho_D^2 [c] \quad (18)$$

$$\dot{\rho}_{He3\downarrow} = \rho_{He3} \rho_n [h] + 2\rho_{He3}^2 [3] + \rho_{He3} \rho_D [i] + \rho_{He3} \rho_t ([j]+[k]) \quad (19)$$

$$\dot{\rho}_{p\uparrow} = \rho_D^2[b] + 2\rho_{He3}^2[3] + \rho_{He3}\rho_D[i] + \rho_{He3}\rho_t[k] + \rho_D[\gamma] \qquad (20)$$

$$\dot{\rho}_{p\downarrow} = \rho_p\rho_n[1b] + \rho_p\rho_D[2] + \rho_t\rho_p[g] \qquad (21)$$

$$\dot{\rho}_{n\uparrow} = \rho_D^2[c] + \rho_t\rho_D[d] + \rho_{He3}\rho_t[k] + \rho_D[\gamma] \qquad (22)$$

$$\dot{\rho}_{n\downarrow} = \rho_p\rho_n[1b] + \rho_n\rho_D[f] + \rho_n\rho_{He3}[h] \qquad (23)$$

$$\begin{aligned}\dot{\rho}_{He4\uparrow} = {} & \rho_D^2[a] + \rho_{He3}^2[3] + \rho_t\rho_D[d] + \rho_t\rho_p[g] + \rho_{He3}\rho_n[h] + \\ & \rho_{He3}\rho_D[i] + \rho_{He3}\rho_t\left([j]+[k]\right)\end{aligned} \qquad (24)$$

Consistent with the units in which the reaction rates are tabulated, $s^{-1}(\text{mole/cm}^3)^{-1}$, we work in density units of mole/cm^3. Thus, the RHSs of (14-24) are in mole/cm^3.sec. The one exception is the rate of photodisintegration, reaction [γ], for which the black body photon density is built into the reaction rate, which is thus in units s^{-1}.

The net increase in the density of any species X is simply $\dot{\rho}_{X\uparrow} - \dot{\rho}_{X\downarrow}$. Hence, solving for the densities of all the nuclei at any time is simply a matter of numerically integrating Equs.(14-24) by time stepping. The initial conditions are the known starting densities for protons and neutrons, and the fact that all other species have zero initial densities. A few subtleties are worth noting.

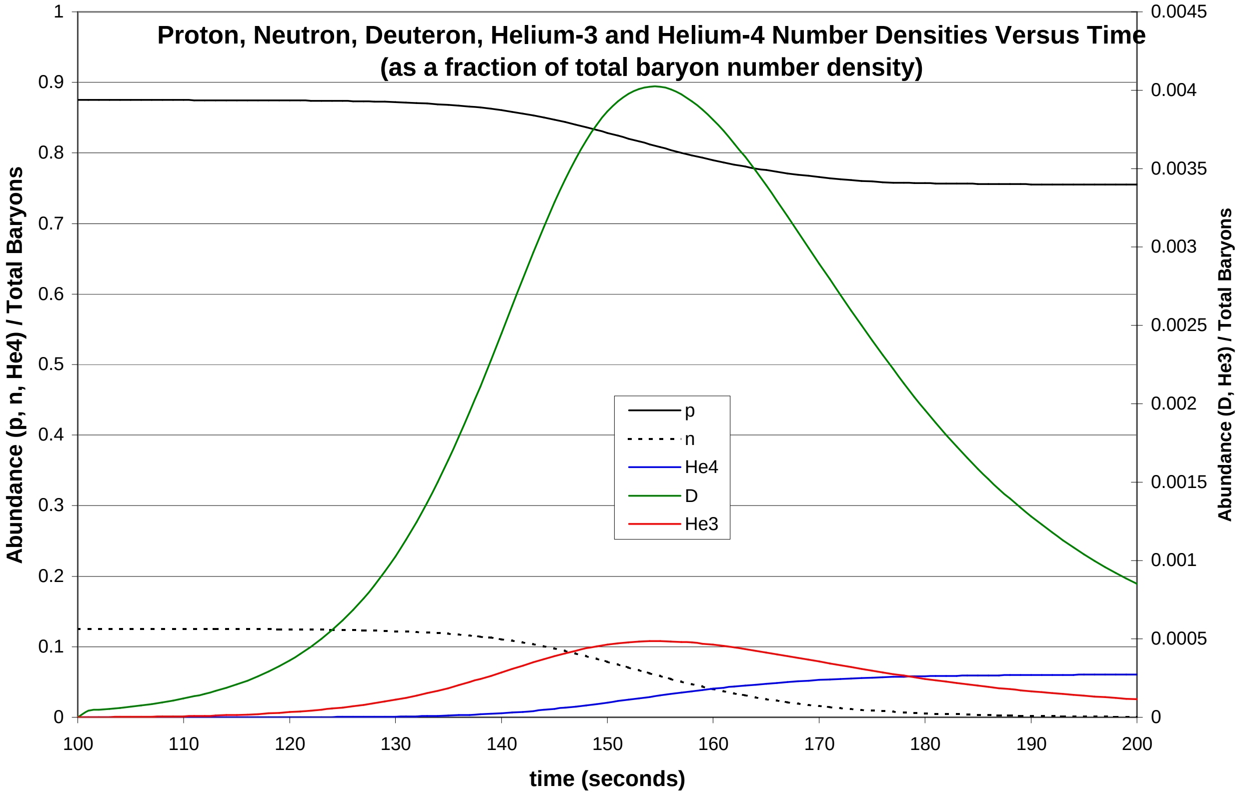
The first is that the time increment has to be small if the solution is to be accomplished in this obvious manner. We found that time steps of around 0.1 milliseconds were needed. Larger increments failed to maintain the required balance between production and consumption reactions. Possibly there is a more sophisticated approach that would use quasi-equilibrium considerations to reduce the number of time steps required. However, our method was workable though it required 4 million time steps to integrate from 100 seconds to 500 seconds.

The second subtlety is that account must be taken of the potential freeze-out of reactions by universal expansion. There is an ambiguity in this concept. Consider a reaction r: a + b → c + d. The expectation time before a given particle 'a' is consumed by this reaction is $1/\rho_b[r]$. Hence, consumption of 'a' would be frozen-out if $\rho_b[r] < 1/2t$. On the other hand, consumption of particle 'b' would be frozen-out if $\rho_a[r] < 1/2t$. As regards production of particles c or d, it is not clear which of the two applies. In our numerical integration we have adopted the interpretation that the production reaction is frozen-out if $\sqrt{\rho_a\rho_b}\cdot[r] < 1/2t$. Unfortunately this can lead to a non-conserved baryon number, because a reaction can be considered as producing products whilst not consuming some of its reactants. The extent of this effect is minor, though (<2%), and was addressed in our program by re-normalising the total baryon number at each step.

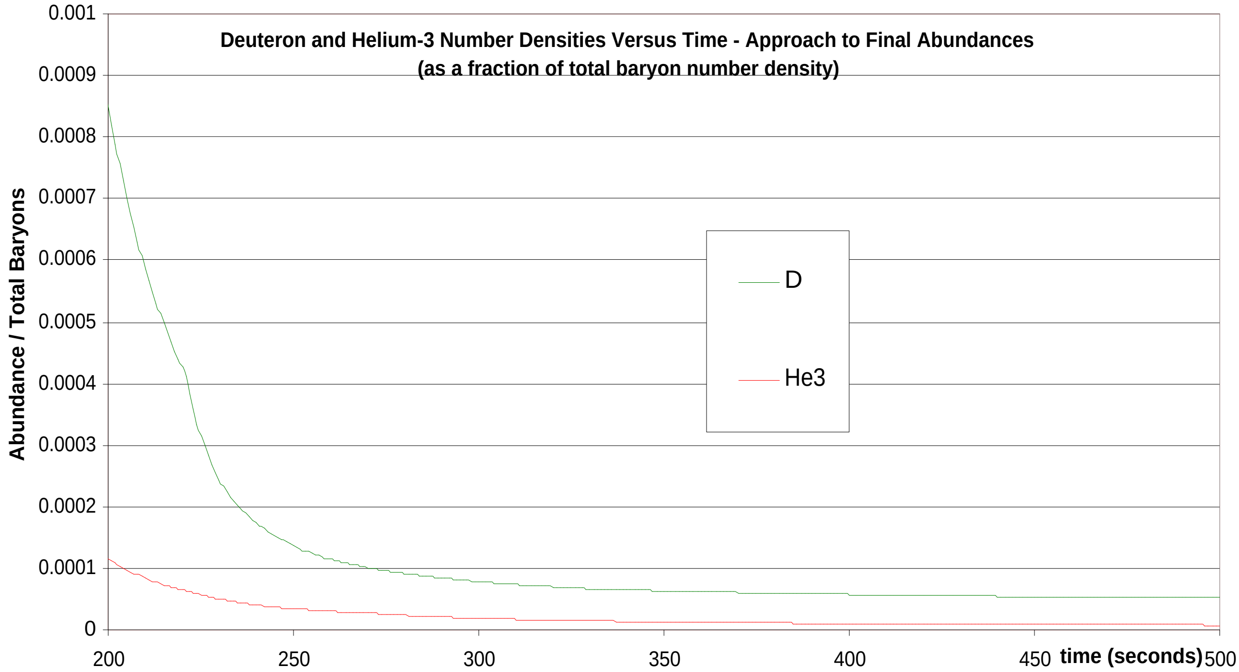
The third factor that must be taken into account is that the universal expansion causes both a change in temperature and a change in density. This is easily accommodated using $T = 1.023x10^{10} / \sqrt{t}$ and $\rho \propto 1/t^{3/2}$.

5. Results

The results are expressed as the abundance of species as a fraction of the total baryon abundance. Over the period between 100 and 200 seconds the results are,



Note that the He3 and D abundances are on a different scale (on the right). Thus, even their peak abundances are two orders of magnitude down on the majority constituents. Their numbers continue to reduce, being close to their frozen-out levels at ~500 secs:-



Thus, the final abundances from our numerical integration are given in the Table below:-

Species	**Abundance as fraction of total baryons**		
	Observed	**Other's BBN Calculations***	**Our BBN Calculation**
p	~0.75	0.755	0.755
n	-	-	5×10^{-15}
He4	0.052 – 0.063	0.0612 – 0.0625	0.0612
D	$10^{-5} – 10^{-4}$	$3 \times 10^{-5} – 8 \times 10^{-5}$	5.4×10^{-5}
He3	$10^{-6} – 3 \times 10^{-5}$	10^{-5}	7.7×10^{-6}

**reported in Rowan-Robinson and/or Guth*

Hence, our results are broadly consistent with BBN calculations in the literature, and also consistent with the observed abundances of p, He4, He3 and D. Note that the neutron density has dropped to extremely low values. In our calculations we also deduced the relative tritium density at 500 seconds to be 5×10^{-18}. However, tritium is radioactive and would not survive long-term in any case (half-life about 12 years).

The advantage of taking the numerical integration approach to the 11 equations, Equs.(14-24), representing the 15 different nuclear reactions, is that it is simple to implement and the complete solution is found. The disadvantage of this approach is that it is not transparent. For this reason we have included a very crude estimate 'by hand' in the Annex. However, the results given in the above Table are our best estimates.

Annex

Crude ‘Hand’ Estimate of He3 and D Abundances

The final abundances of He3 and D occur when the reactions producing and consuming them have ceased to operate. To make our crude estimate we concentrate on the freeze-out by universal expansion of the deuteron consumption reactions. These are reactions 2, a, b, c, d, f and i. Reaction a has a negligible rate and can be ignored. Similarly, reactions 2 and f have rates which are far slower than reactions b, c, d and i and can also be ignored. Reaction d requires tritium, and we have seen that the density of tritium is always very low, hence reaction d can also be ignored. We are left with reactions b, c and i.

From Section 2 we expect the reactions to be nearing completion by 290 seconds. At this time the temperature is 6.0 x 10^8 K and the sum of the reaction rates of b and c is 7.5 x 10^6 $s^{-1}(mole/cm^3)^{-1}$. Both reactions b and c involve two deuterons. Hence, reactions b+c will be frozen out as regards consumption of deuterons if ρ_D x 7.5 x 10^6 < 1/2t. This suggests freeze-out of D-consumption by b+c for ρ_D < 2.3 x 10^{-10} mole/cm^3. The total baryon density at this time is 3.8 x 10^{-6} mole/cm^3 so freeze out occurs for ρ_D/ρ_b < 6 x 10^{-5}. This is in good agreement with the result of the numerical integration, above. However, note that there is a degree of arbitrariness about the time (temperature) chosen.

We must also ensure that deuterons are not still being consumed by reaction i either. The rate of reaction i at 290 seconds is 3.6 x 10^7 $s^{-1}(mole/cm^3)^{-1}$. Hence, reaction i will be frozen out as regards consumption of deuterons if ρ_{He3} x 3.6 x 10^7 < 1/2t. This suggests total freeze-out of deuteron consumption if ρ_{He3} < 4.8 x 10^{-11} mole/cm^3, i.e., ρ_{He3}/ρ_b < 1.2 x 10^{-5}. This is also in rough agreement with the results of the numerical integration, above.

These arguments are not rigorous, of course. They are intended only to illustrate why the final abundances of D and He3 are of the order they are, namely about four or five orders of magnitude less than the dominant components, p and He4.