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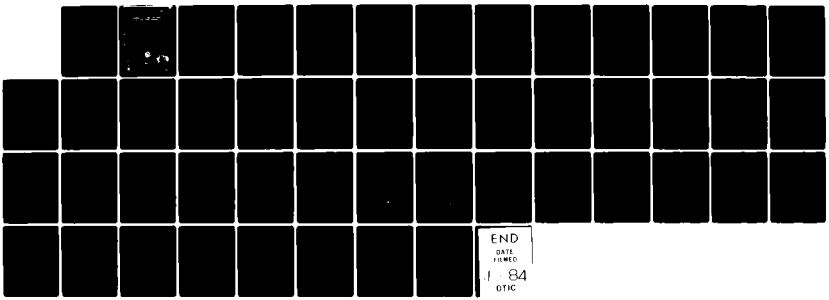

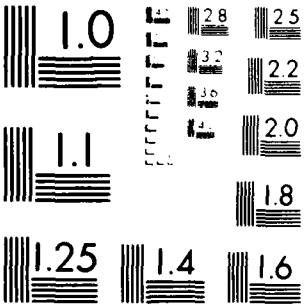

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20 ABSTRACT (Continue on reverse side if necessary and identify by block number)

~~We~~ present simulation results for a large uranium gas release in the ionosphere at an altitude of 200 km. The purpose of such an experimental release would be to study infrared emission line strengths and spectra of uranium oxides after a nuclear explosion. The simulation shows that the release would have high ion densities ~~$\sim 10^8$ cm^{-3}~~, that it would have a radius of about half a kilometer perpendicular to the geomagnetic field, and that it would spread to a few kilometers along the field. ~~We~~ The also demonstrate the complete oxidation of U to UO_2 would require tens of seconds.

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UO2(+)

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SIMULATION OF A URANIUM VAPOR RELEASE IN THE HIGH ALTITUDE ATMOSPHERE

I. Introduction:

High altitude nuclear explosions can lead to greatly enhanced infrared radiation in the earth's atmosphere and can thereby have a deleterious effect on defensive infrared systems. This enhanced infrared radiation has a number of sources: direct plasma radiation from the nuclear burst created plasma; creation of increased densities and/or increased temperatures of natural atmospheric infrared radiators such as hydroxyl, nitrogen oxides and carbon oxides; and also infrared radiation of weapon and vehicle debris species which are vaporized in the explosion. Recently it has been recognized that uranium and its oxides are likely to be the dominant infrared active species at 10 minutes and later following a high altitude nuclear detonation (Armstrong, 1981).

The Defense Nuclear Agency has an interest in developing methods to predict the infrared radiation after a high altitude nuclear event. Armstrong points out those areas where there is a severe lack of knowledge required to make accurate predictions. In order to measure the spectral lines and the strength of long wavelength infrared emission it is expected that fairly large releases of uranium vapor will be necessary in the earth's high atmosphere. Only after such measurements are made will accurate predictions become possible. With this requirement in mind, we have considered the scenario originally described by Reidy (1980) involving the prompt deposition of 2 kg of uranium vapor at an altitude of 200 km. Current experimental release techniques are short of being capable of this rapid a deposition by orders of magnitude.

In this memorandum, we present results for the temporal evolution of a uranium vapor release at approximately 200 kilometer altitude in the earth's atmosphere. The results are obtained by numerical simulations using a simple model and can be used to plan such an experimental release. The results describe both the chemical and hydrodynamic evolution for one experimental scenario for time periods of a few tens of seconds. We predict a uranium ion cloud extended along the field but narrow perpendicular to the earth's magnetic field. The ion densities are high for minutes after release with the

Manuscript approved August 18, 1983.

ions, UO^+ and UO_2^+ , formed in shells around the release point. The time scale for complete oxidation of U to UO_2^+ is demonstrated to be a few tens of seconds.

II. Simulation Model:

We consider a simple one-dimensional model of the uranium release. The temporal evolution of each species, denoted α, is described by equation 1.

$$\frac{\partial n_\alpha}{\partial t} = \frac{\partial n_\alpha}{\partial t}\,\text{hydro} + \frac{\partial n_\alpha}{\partial t}\,\text{diff} + \frac{\partial n_\alpha}{\partial t}\,\text{chem} \tag{1}$$

The first term on the right is the change in the concentration from hydrodynamic transport. The second term describes diffusion of ions through ions and neutrals through neutrals. The third term treats chemical transformation of the individual species.

The hydrodynamic transport of ions and neutrals is done separately. The transport equations are:

continuity

$$\frac{\partial \rho_s}{\partial t} = -\nabla\cdot(\rho_s \underline{v}_s), \tag{2}$$

momentum

$$\frac{\partial \underline{v}_s}{\partial t} = -(\underline{v}_s\cdot\nabla)\underline{v}_s - \frac{1}{\rho_s}\nabla(p_s + q_s) - \sigma p_t(\underline{v}_s - \underline{v}_t) \tag{3}$$

and energy

$$\frac{\partial p_s}{\partial t} = -\nabla\cdot(p_s\underline{v}_s) - (\gamma - 1)\,(p_s + q_s)\,\nabla\cdot\underline{v}_s$$

$$-\sigma\rho_s\rho_t(T_t - T_s) + (\gamma-1)\,\frac{\sigma\rho_s\rho_t}{(\rho_s + \rho_t)^2}\,\rho_s(\underline{v}_s - \underline{v}_t)^2 \tag{4}$$

Here s denotes either the ions or the neutrals and t denotes the other. The symbols ρ ,$\underline{v}$, p, T, and q are density, flow velocity, pressure, temperature,

and artificial viscosity respectively. γ is the ratio of specific heats and σ the collisional coefficient of friction.

In this simple one dimensional model of transport we treat two specific cases; transport perpendicular and transport parallel to the ambient geomagnetic field. Perpendicular to B the neutrals are transported spherically and the ions are frozen to the unmoving field. Parallel to B, the neutrals are transported spherically and the ions are transported along a cartesian axis parallel to the field. The two cases of the simple one-dimensional model should give reasonable estimates for the size of a release cloud in the atmosphere. Since the transport model allows for diffusion between ions and neutrals our diffusion model only needs to consider neutrals and ions diffusing through themselves.

The diffusion equation in a multi constituent gas can be expressed (Burgers 1969)

$$\sum_{\lambda} \rho_\alpha \rho_\beta \sigma_{\alpha\beta} (\underline{v}_\alpha - \underline{v}_\beta) = T(\nabla \rho_\alpha - \frac{\rho_\alpha}{\rho} \nabla \rho). \tag{5}$$

where ρ is the total density. An exact solution for diffusion can be obtained by inversion of (5) and substitution of the species velocities into a set of coupled continuity equations for each specie. For our model here however we approximate (5) and obtain a decoupled set of continuity equations. We assume $\sigma_{\alpha\beta} = \sigma$, a constant, which allows us to express the effects of diffusion as

$$\frac{\partial \rho_\alpha}{\partial t} = -\nabla \cdot (\kappa \nabla \rho_\alpha / \rho), \tag{6}$$

where κ is a diffusion coefficient depending on σ . We have tested this simplified diffusion model and have obtained reasonable results. The simplification of diffusion, while not totally accurate, yields results which are within a factor of two.

The effects of chemistry on the species are computed in a series of rate equations

$$\frac{\partial n_\alpha}{\partial t} = k_{st} n_s n_t. \tag{7}$$

The reactions of concern and their rate coefficients, k_{st}, are shown in Table 1 which are taken from Armstrong (1981) and Archer (1982).

The final part of the model is the specification of the neutral atmosphere. We have taken species concentrations and a temperature appropriate to moderate solar activity, daytime, 200 km altitude conditions; they are $[O] = 4.4 \times 10^9\ cm^{-3}$, $[N_2] = 4.2 \times 10^9\ cm^{-3}$, and $[O_2] = 2.6 \times 10^8 cm^{-3}$. The neutral atmospheric temperature is 0.1 ev.

III. Results:

We have solved the model equations 1,2,3,4,6, and 7 for a uranium vapor release at 200 km altitude in the atmosphere. We have assumed a prompt release of 2 kg of atomic uranium, approximately $5. \times 10^{22}$ atoms. The temperature of the uranium vapor is taken as 0.276 ev. Three sets of solutions were obtained with the diffusion coefficient, κ, as a parameter to study the effects of diffusion on the release evolution. In the first, or nominal, case κ was taken as 0.1 km^2/sec, a nominal diffusion coefficient at 200 km altitude. For an appropriate gradient scale length of 100 m the diffusion velocity is 100 m/sec. This value is about 17% of the sound speed at that altitude. We have also obtained results for diffusion coefficients 1/3 and 3 times the nominal value. The slower diffusion rates lead to very slow oxidation of the uranium vapor and are therefore uninteresting. In the following sections we show results for nominal diffusion and faster diffusion.

Figures 1 through 14 show results for the simulation perpendicular to the geomagnetic field with nominal diffusion. Figure 1 shows the initial conditions of the release. The vertical axis plots the logarithm to the base 10 of the gas concentration while the horizontal axis measures radius of the release in km. The uranium vapor has a radius of 200 m and has displaced the ambient atmospheric species. We have tested a number of initializations and find that the results after a few seconds are insensitive to details of the initial conditions.

Figures 2, 3, and 4 show the neutral gas concentration at 2, 5, and 10 seconds respectively. Initially both atomic and molecular oxygen are burned out of the release cloud in oxidizing the uranium gas. The atomic oxygen is able to diffuse into the cloud by about 5 seconds but the molecular oxygen continues to be consumed as it diffuses in for times longer than 10 seconds.

Table 1

Chemical Reaction Rate Coefficients

(1)	$U + O \rightarrow UO^+ + e^-$	5×10^{-10} cm^3/sec
(2)	$U + O_2 \rightarrow UO_2^+ + e^-$	3.8×10^{-12} cm^3/sec
(3)	$U + O_2 \rightarrow UO + O$	1.8×10^{-10} cm^3/sec
(4)	$UO + O \rightarrow UO_2^+ + e^-$	4×10^{-10} cm^3/sec
(5)	$UO + O_2 \rightarrow UO_2 + O$	2×10^{-9} cm^3/sec
(6)	$UO^+ + O_2 \rightarrow UO_2^+ + O$	4×10^{-9} cm^3/sec

The different behaviour of atomic and molecular oxygen is due primarily to their different concentrations in the ambient atmosphere; there just is not enough molecular oxygen around to rapidly fully oxidize the cloud.

The resulting ion cloud concentrations are presented in Figures 5 through 11 for post release times of 2 to 50 seconds. The UO^+ component forms in a shell like structure at a radius of about 200 meters from the release point. The shell is formed at a burning front between outward diffusing uranium vapor and inward diffusing atomic oxygen, and the ions are frozen in the geomagnetic field at their point of oxidation. The initial oxidation of uranium gas to UO^+ is complete by 5 seconds. Further burning of UO^+ to UO_2^+ by molecular oxygen then takes place in an outer shell which slowly moves inward as unconsumed molecular oxygen is able to diffuse inward. The complete oxidation of uranium vapor to UO_2^+ takes between 40 and 50 seconds. The final ion densities of 10^{11} cm^{-3} in the shell are higher than would occur in an actual release because this one-dimensional model does not allow for diffusion parallel to the magnetic field. From studying our one dimensional parallel release results we would expect the maximum ion cloud densities to be about 10^9 cm^{-3} for this release.

Figures 12, 13, and 14 show the results for UO^+, UO_2^+, and O_2 concentrations respectively in a different graphical format. We have plotted contours of concentration versus radius and time after release. Here the shell structure of the ion cloud is clearly seen. The UO^+ forms a shell at 200 meters radius immediately after release. The UO_2^+ shell initially forms at about 400 meters and gradually builds inward as oxidation takes place. We are also able to see the cavity formed in the ambient O_2 which is only slowly filled by diffusion from the outside.

A similar set of results for the evolution of the uranium release parallel to the geomagnetic field is shown in Figures 15 through 24. The initial conditions, which are identical to the previous case are shown in Figure 15; note the change in scale on the horizontal axis. The neutral concentrations for 2, 5, and 10 seconds after release are shown in Figures 16, 17, and 18 respectively. The ion concentrations for the same time intervals after release are shown in Figures 19, 20, and 21. The qualitative nature of the temporal and spatial evolution is like that discussed previously for the perpendicular release. The primary difference in the results is that here the

ion cloud is able to readily diffuse outward. This parallel diffusion allows the UO_2^+ to become very extended along the geomagnetic field. The UO^+ is however still confined to the release region as it is consumed by oxidation by molecular oxygen as it attempts to diffuse parallel to the magnetic field.

Figures 22,23 and 24 show contours of UO^+, UO_2^+, and O_2 concentration respectively for the parallel simulation. Again the results are similar to those for the perpendicular simulation. The formation of an ion cloud shell about the release point is again clearly seen. The shell is broader in this case, and for UO_2^+ diffusion outward is very noticeable. The molecular oxygen is depleted in the release location, and for this case the burned out region is very much larger as the ions diffuse outward.

The results for the uranium release simulations with 3 times faster diffusion are shown in Figures 25 through 28. The initial conditions are the same as used for normal diffusion. Figures 25 and 26 present results of the perpendicular simulation 10 seconds after release for the neutrals and ions respectively. Figures 27 and 28 show results for the parallel simulation. The results in both instances are qualitatively similar to those represented previously. The major quantitative differences are a more rapid oxidation of UO^+ to UO_2^+ allowed by faster diffusion of O_2 into the ion cloud, and for the parallel case, a more rapid diffusion of UO_2^+ along the geomagnetic field. Nevertheless the time scale for the complete oxidation of U to UO_2^+ is still greater than 10 secs.

IV. Conclusions

The results of the numerical simulation of a uranium vapor release at about 200 km altitude have demonstrated a very consistent and understandable morphology. For the 2 kg prompt release considered here, it is clearly demonstrated that the uranium vapor will completely burn out the molecular oxygen of the ambient neutral atmosphere. Moreover diffusion of molecular oxygen from outside into the release cloud is not sufficient to rapidly oxidize the cloud to its final state, UO_2^+. We have shown that the time scale for complete oxidation is a few tens of seconds.

It might be thought that increasing the altitude of release would alleviate the slow oxidation of the cloud owing to faster diffusion rates. Unfortunately this is probably not the case since the atmospheric molecular

oxygen density decreases rapidly with altitude and the burn out would be more severe. It would appear that the only solution to the slow oxidation problem would be to release the uranium vapor gradually. However, in this case one would not have a compact cloud for measurement but would have a long thin trail of oxidized uranium ions across the sky.

The morphology of the release simulated here has a clearly defined shell structure. The ion cloud is also greatly extended along the geomagnetic field. At early times after release the ions form a double shell with UO_2^+ ions forming outside the UO^+ shell. At later times there is a single shell of UO_2^+ ions with a diameter of about 1 km perpendicular to the magnetic field and a length along the field of more than 10 km. The simulation indicates that the ion density in the shell can be expected to be 10^8 to 10^9 cm^{-3}. This is a very high density when compared to the well studied barium vapor release where the ion densities are normally 2 orders of magnitude lower.

These very high ion densities can have important implication for gradient drift structuring for the uranium release ion cloud. For barium releases, it has been demonstrated that ion clouds which have a large conductivity ratio compared to the background ionosphere form striations very slowly (Linson, 1975). Therefore, we would expect that a uranium vapor release would create a slowly structuring ion cloud. This situation may be somewhat alleviated by conducting the uranium release during daytime with higher ambient ionospheric conductivities. However, on balance the uranium ion cloud should only slowly form striations.

In summary, we conclude that a prompt uranium vapor release would result in a UO_2^+ ion cloud in a few tens of seconds. The ion cloud would have a shell like structure and be compact perpendicular to the magnetic field and very elongated along the field. The ion concentrations would range from 10^8 to 10^9 cm^{-3} and would develop striated structure very slowly.

Acknowledgments

This work was supported by the Defense Nuclear Agency.

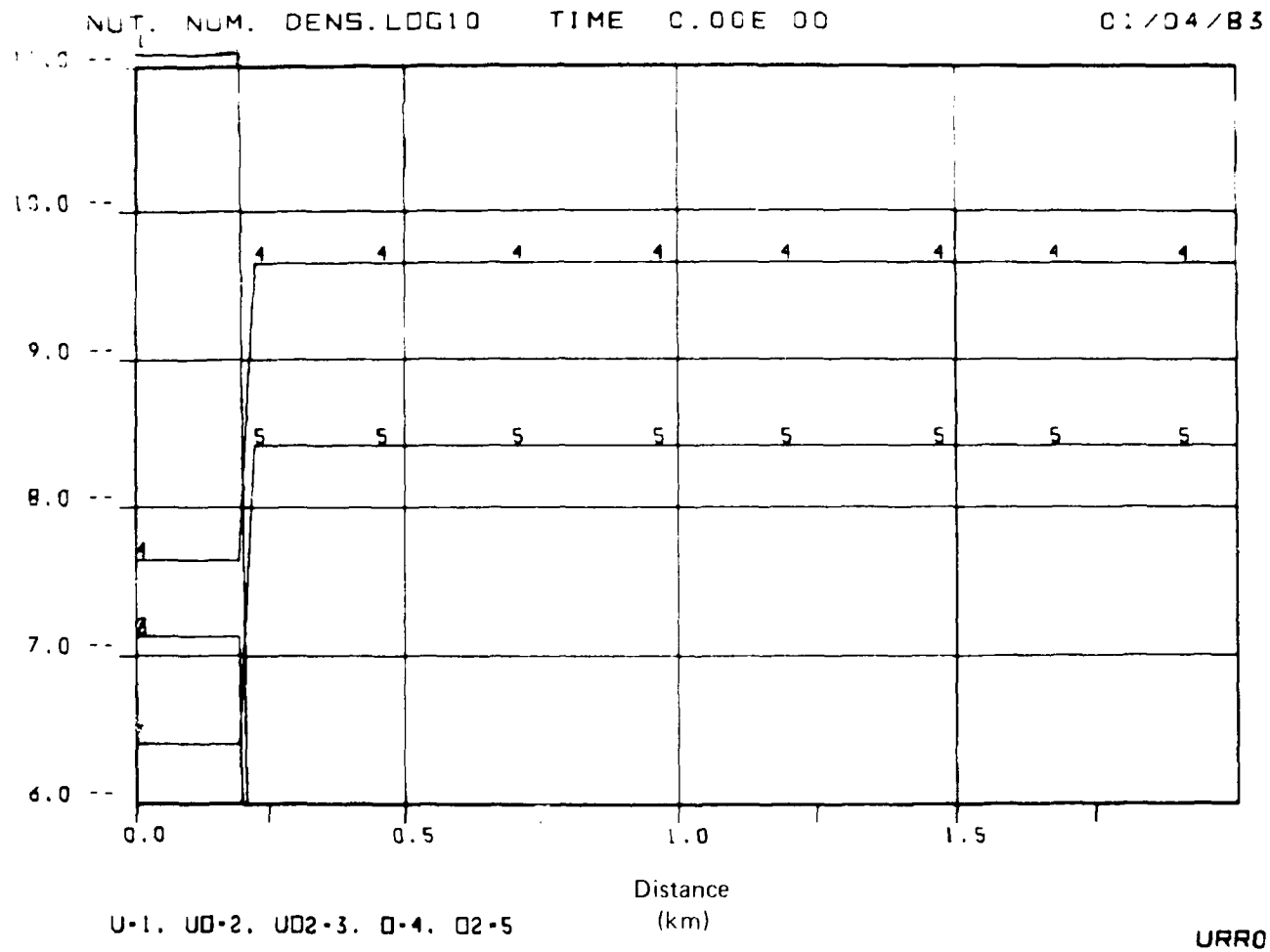

Figure 1. Initial conditions for simulation perpendicular to the geomagnetic field and nominal diffusion. Logarithm to base 10 of gas concentration in cm^{-3} are shown for U, UO, UO_2, O, and O_2 versus radius from burst point.

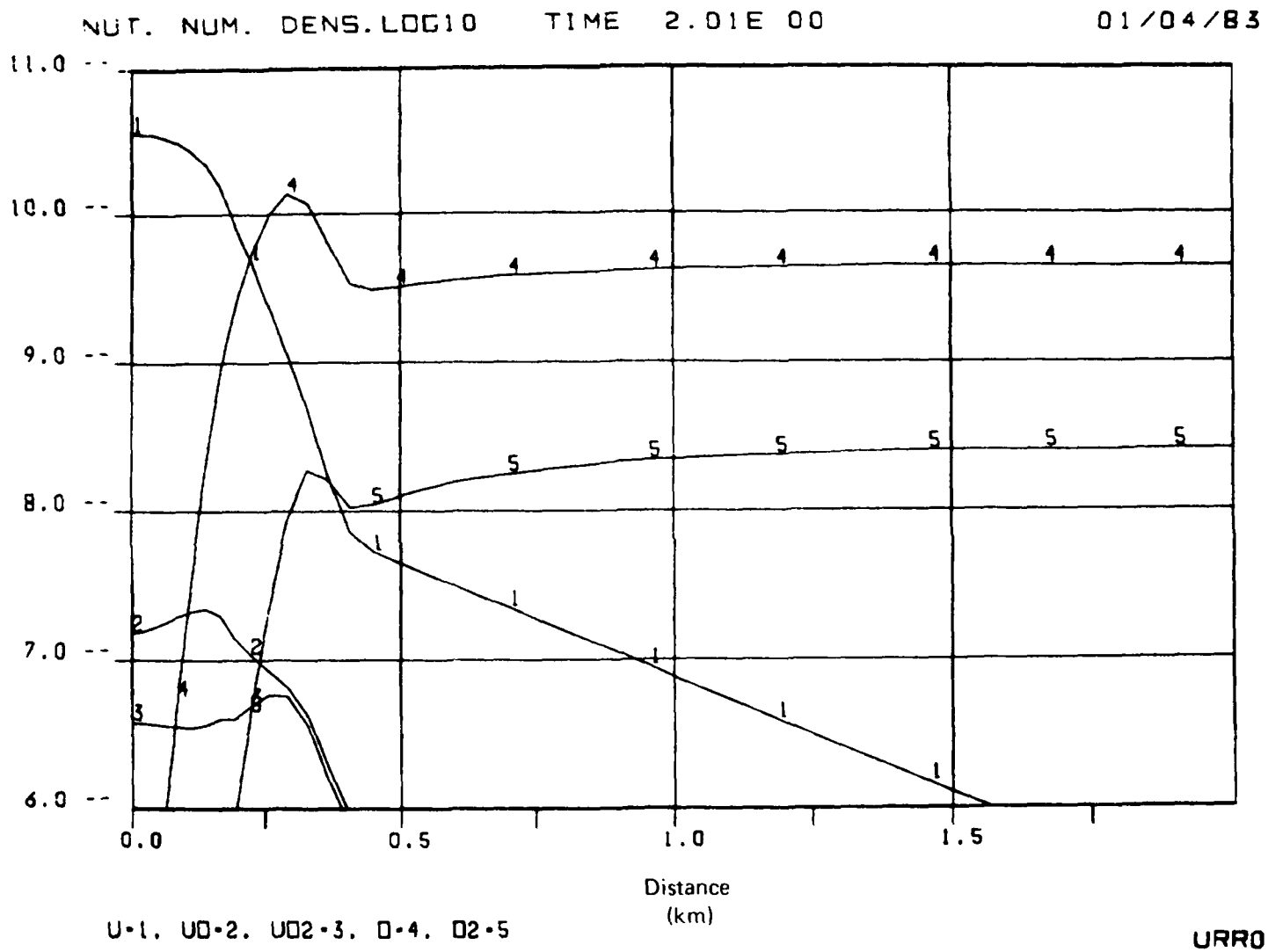

Figure 2. Neutral gas concentration at 2 seconds after release.

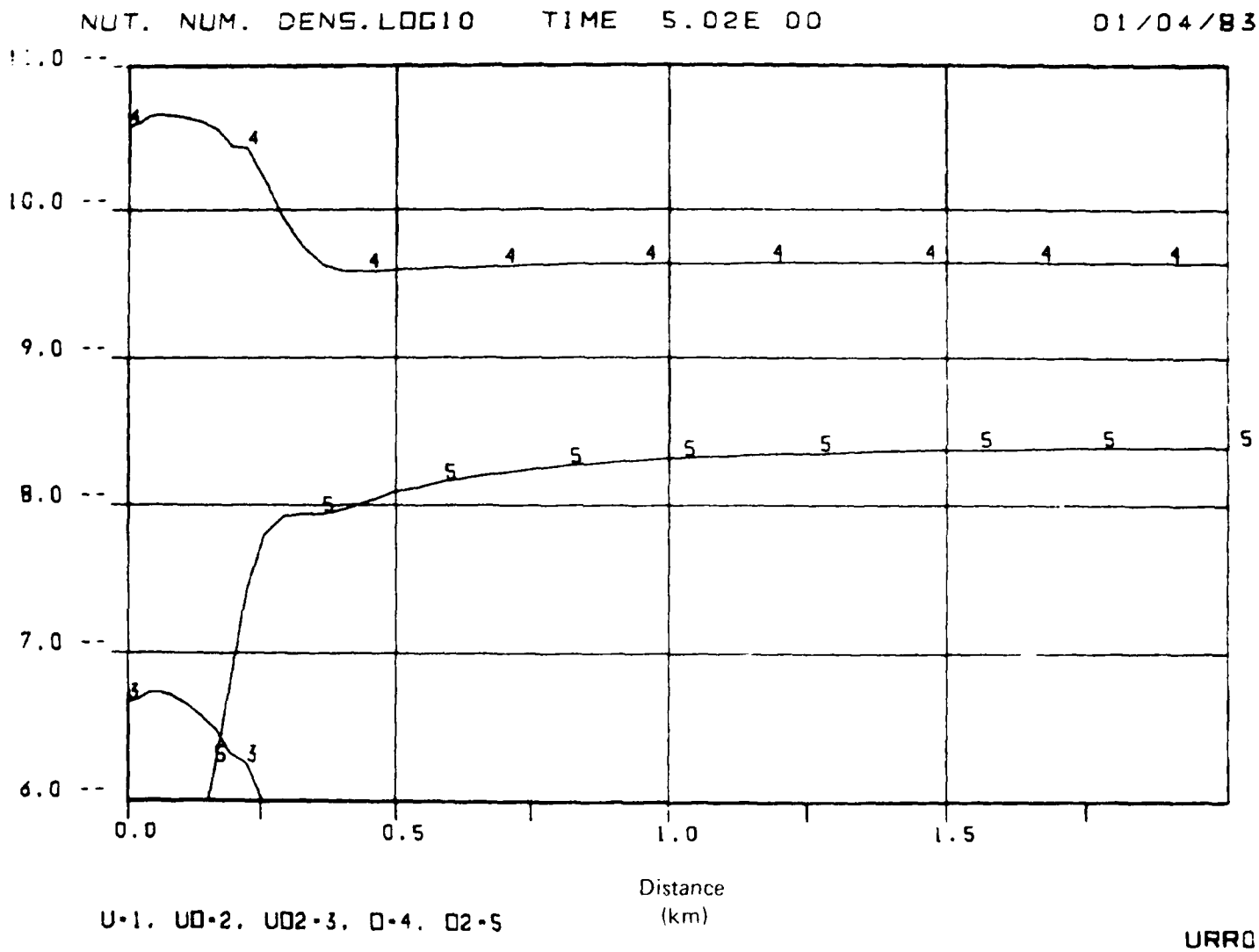

Figure 3. Neutral gas concentrations at 5 seconds after.

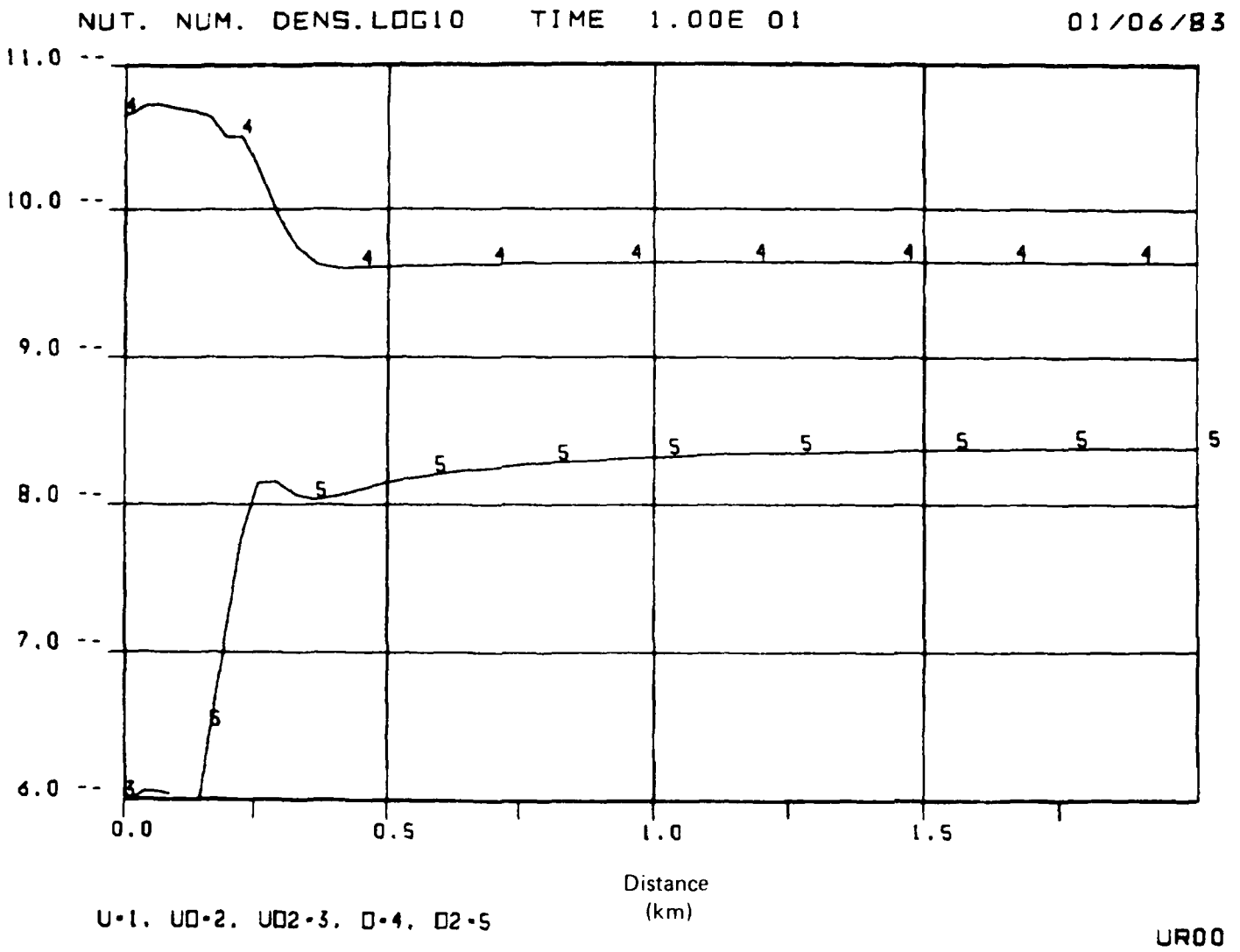

Figure 4. Neutral gas concentrations at 10 seconds after release.

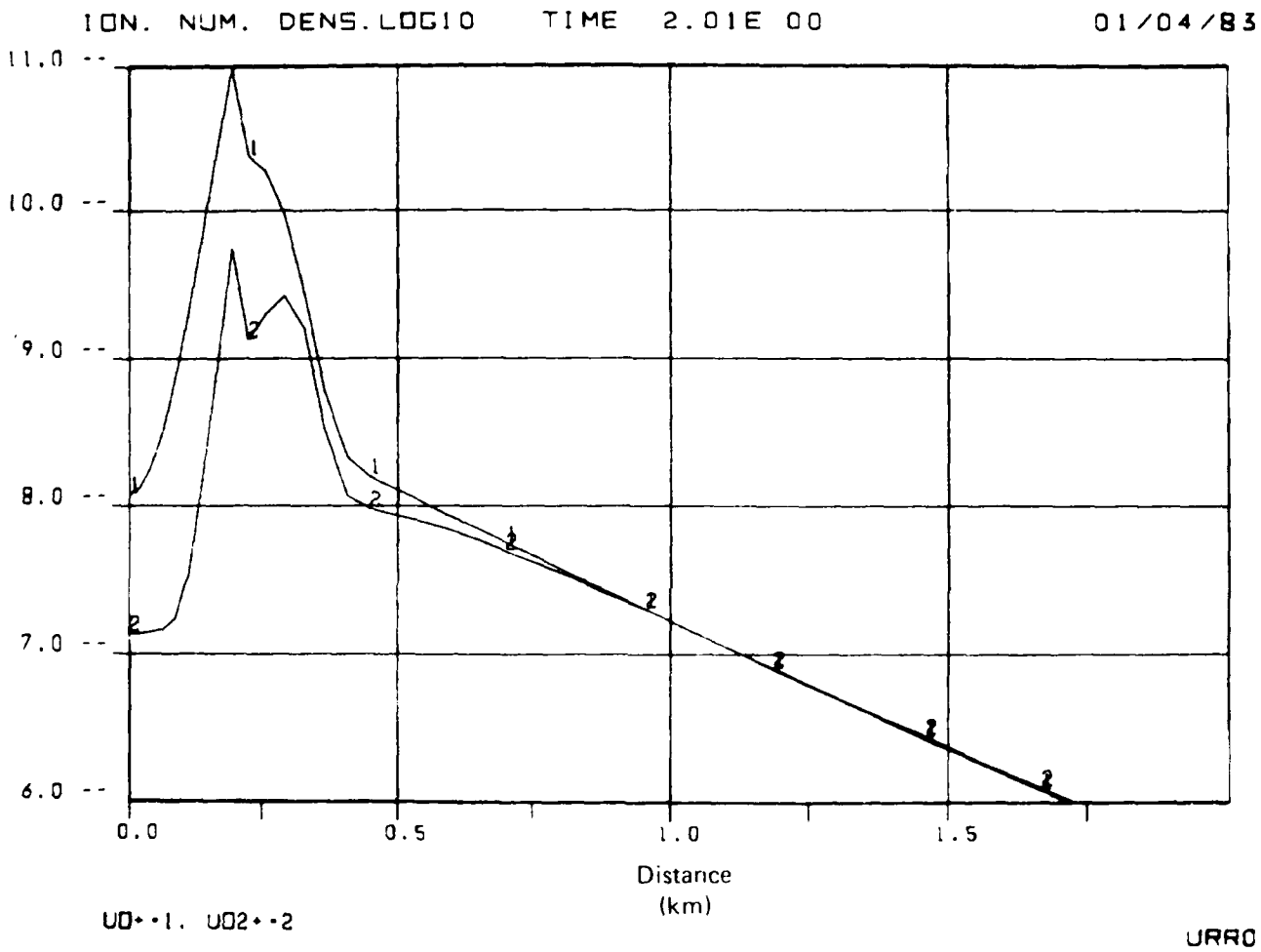

Figure 5. Ion gas concentrations at 2 seconds after release. Logarithm to base 10 of ion concentrations in cm^{-3} are shown for UO^+ and UO_2^+ versus distance from burst point perpendicular to geomagnetic field.

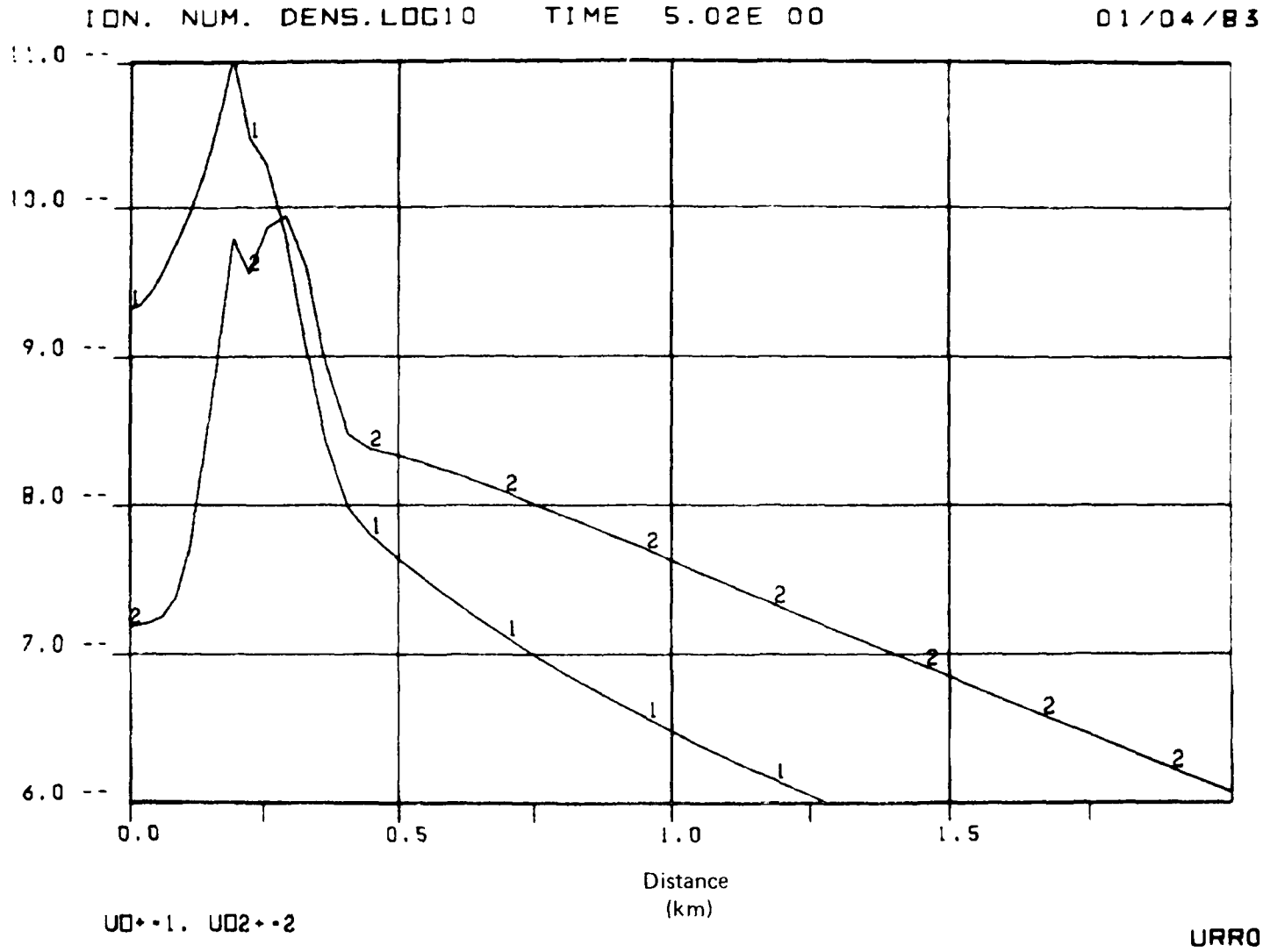

Figure 6. Ion gas concentrations at 5 seconds after release.

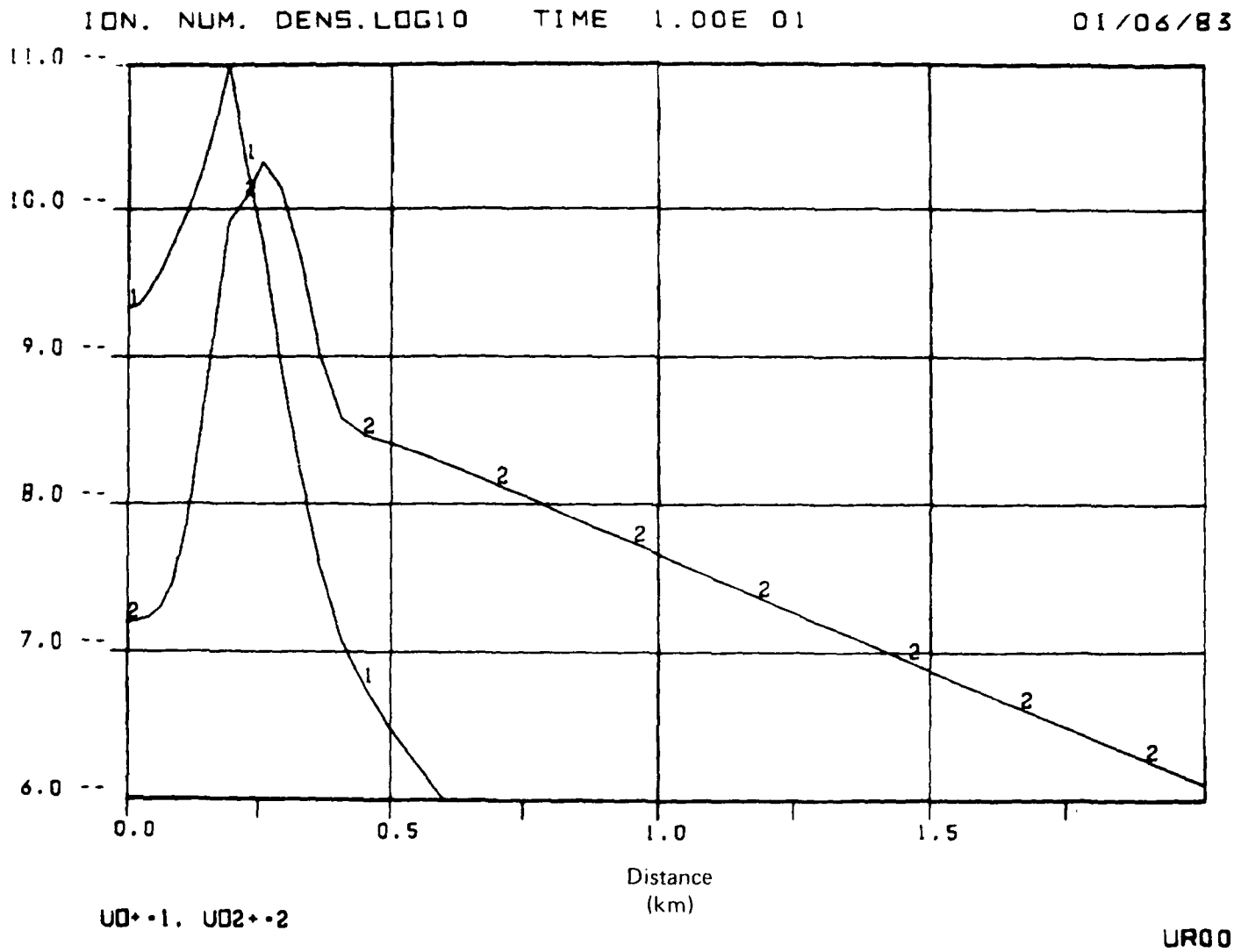

Figure 7. Ion gas concentrations at 10 seconds after release.

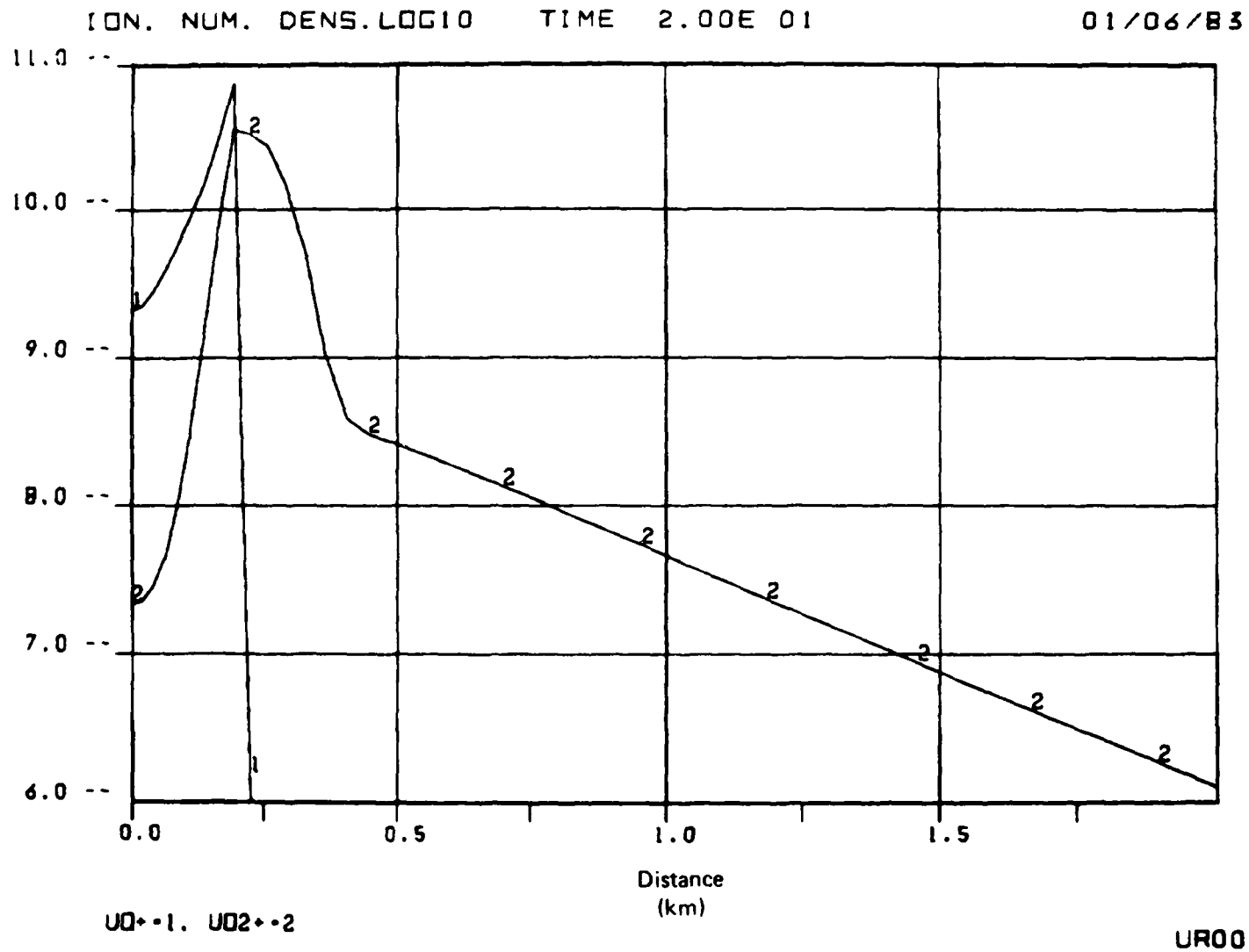

Figure 8. Ion gas concentrations at 20 seconds after release.

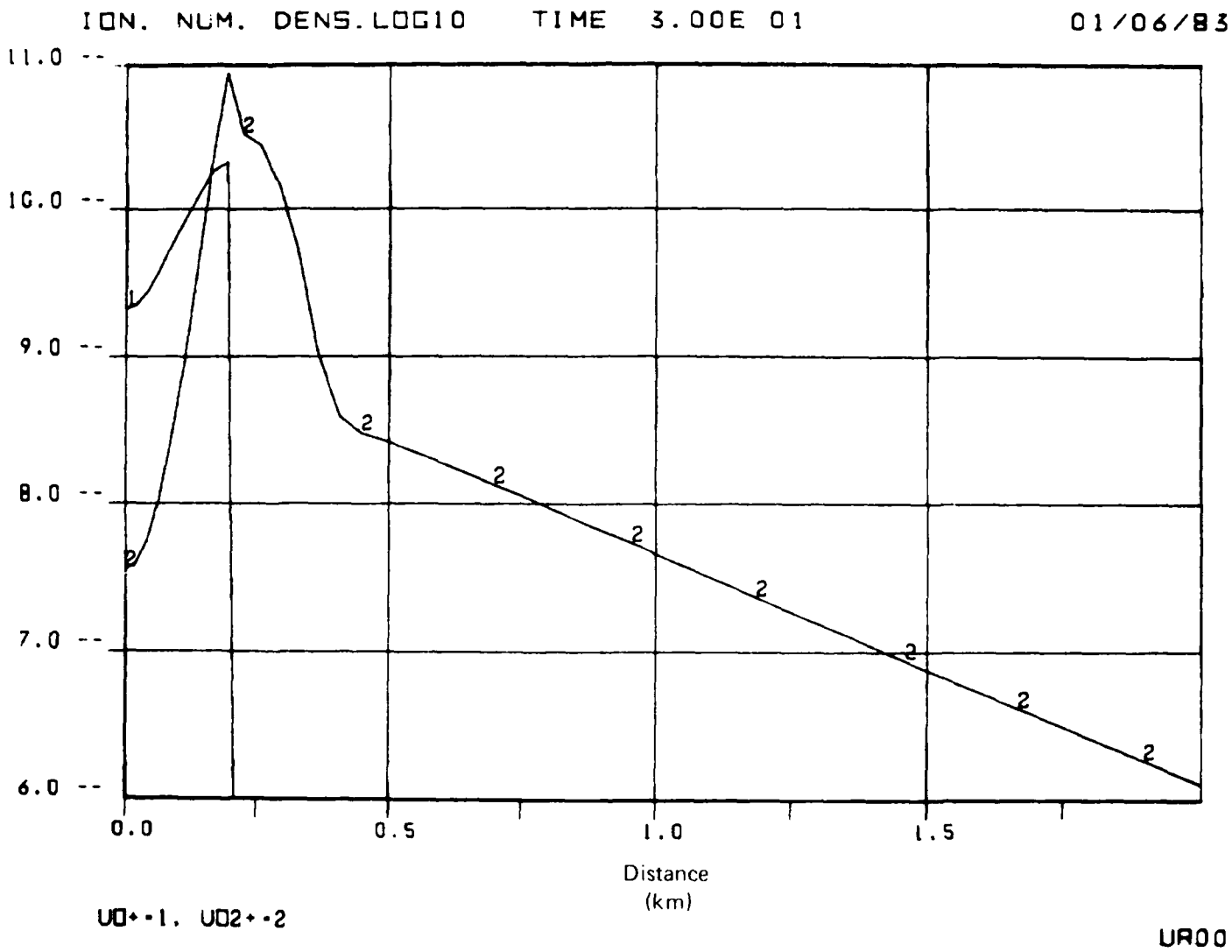

Figure 9. Ion gas concentrations at 30 seconds after release.

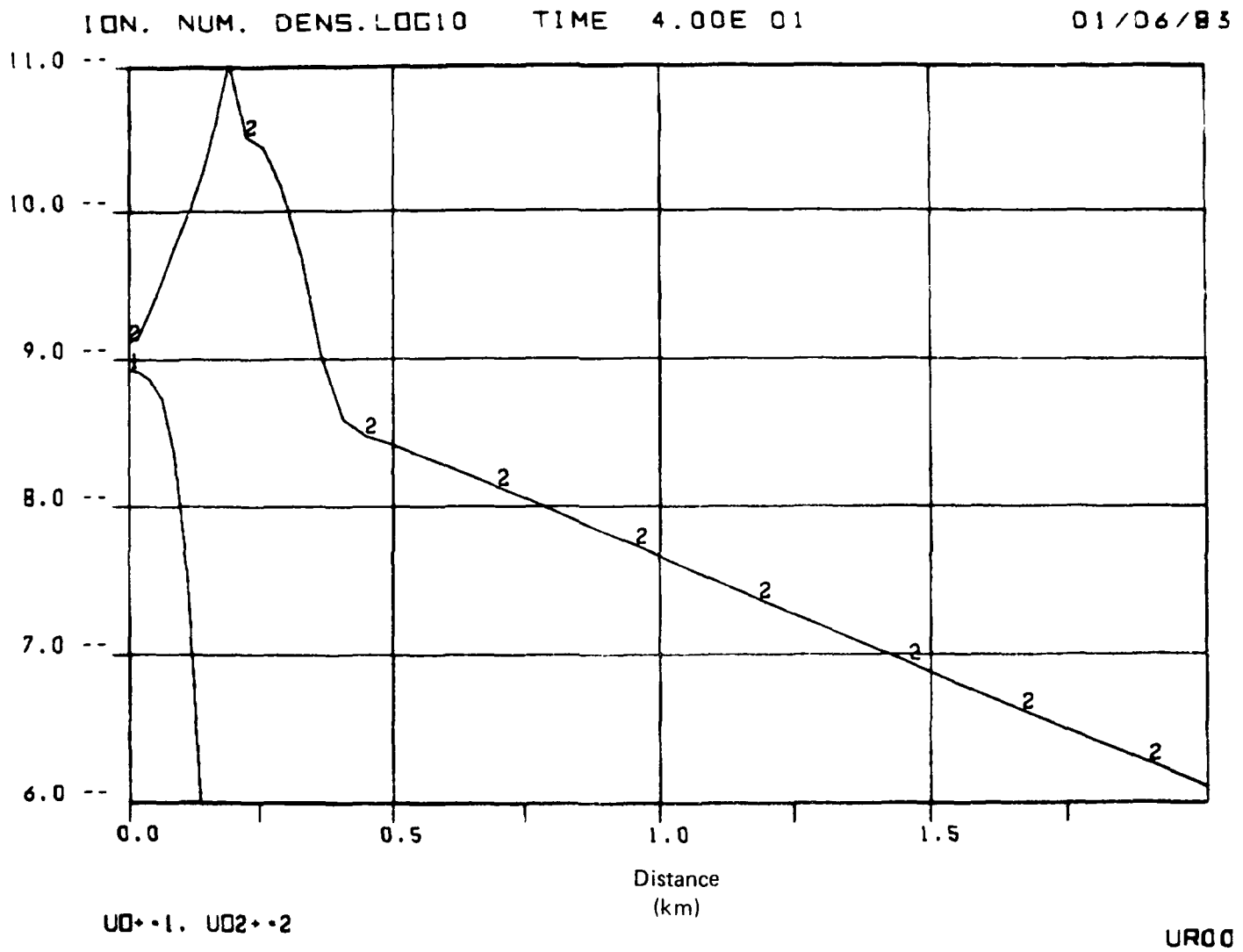

Figure 10. Ion gas concentrations at 40 seconds after release.

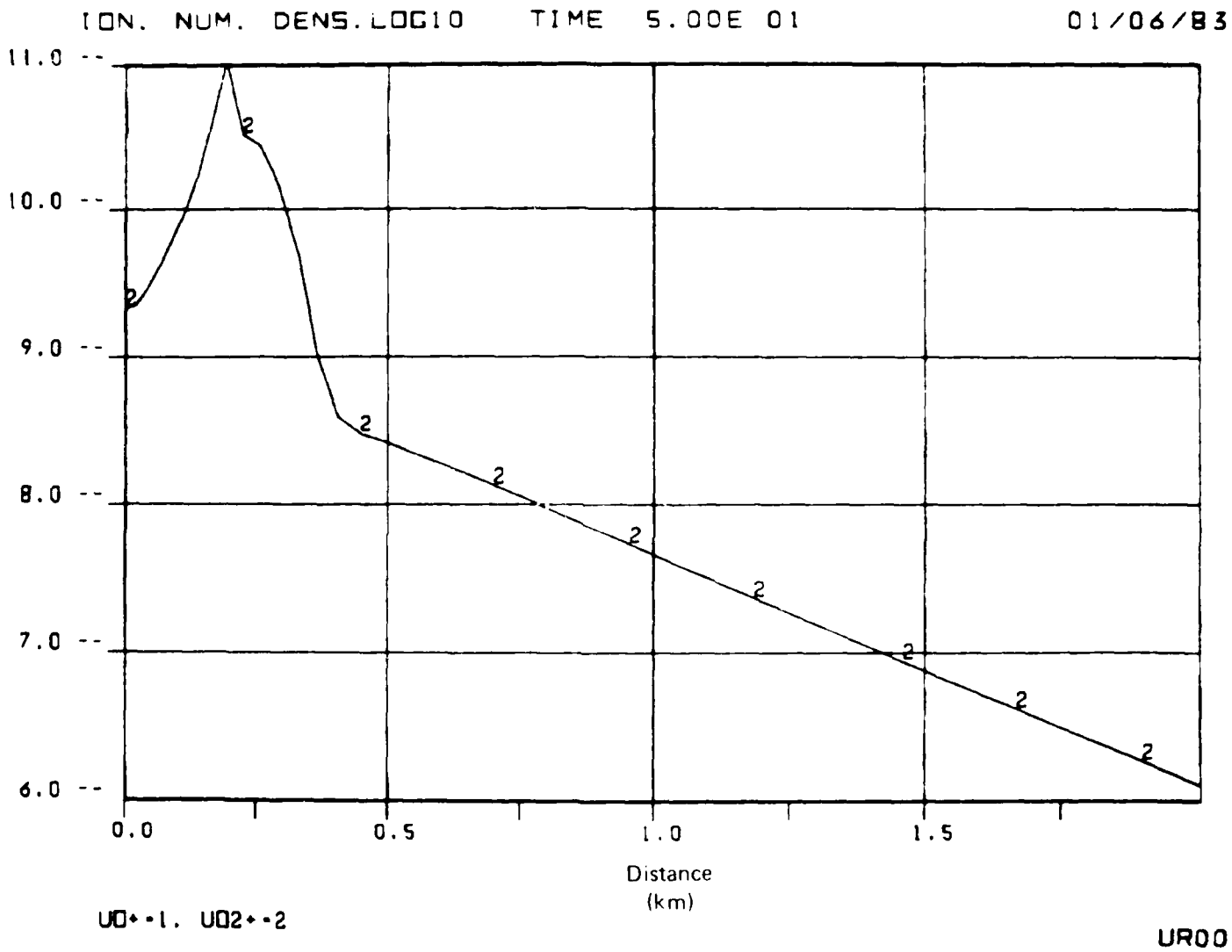

Figure 11. Ion gas concentrations at 50 seconds after release.

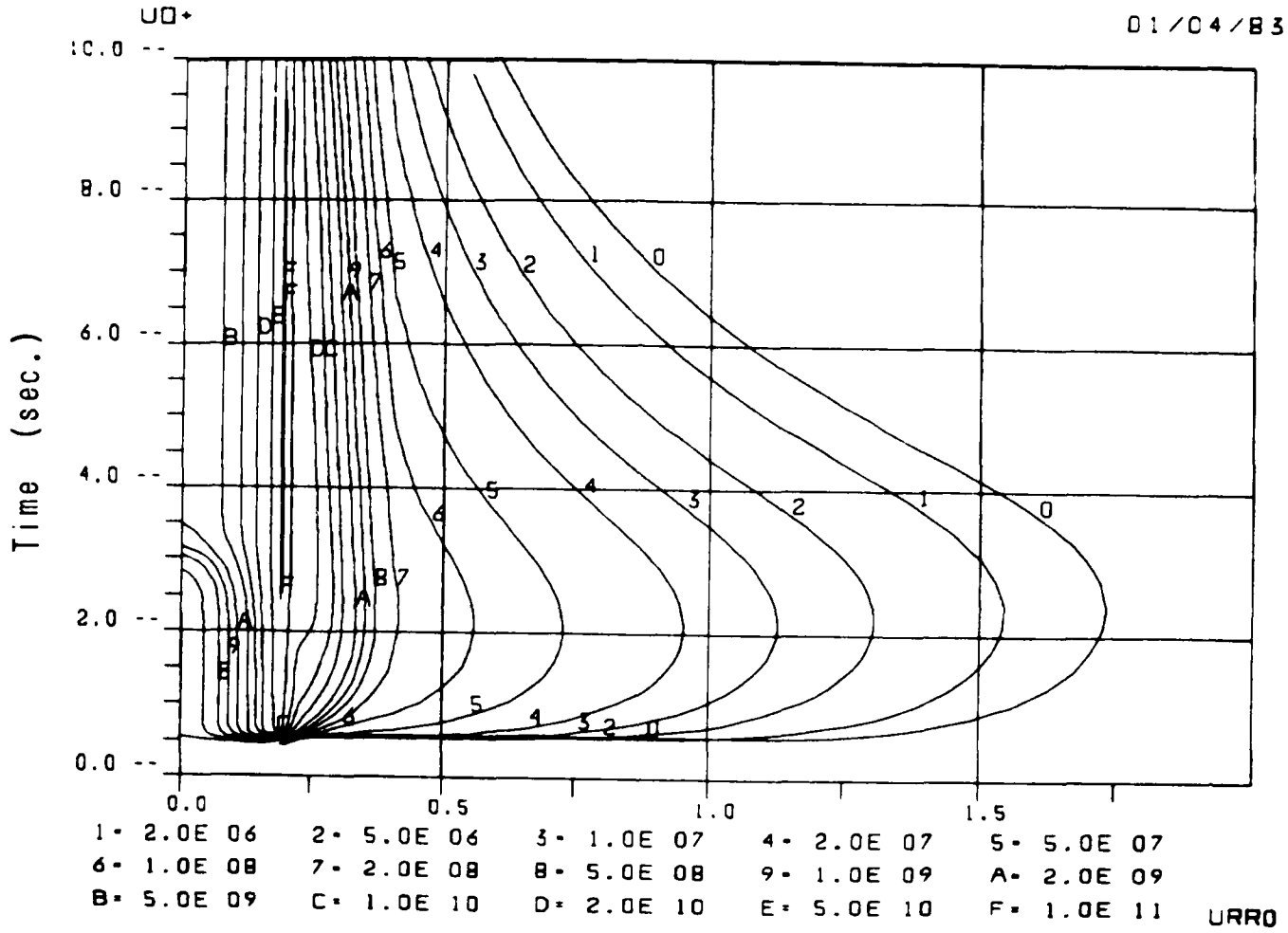

Figure 12. UO^+ ion concentration contours versus time and distance from release point. Contours are in cm^{-3}. Notice shell formation at 0.2 km which only gradually decays in time.

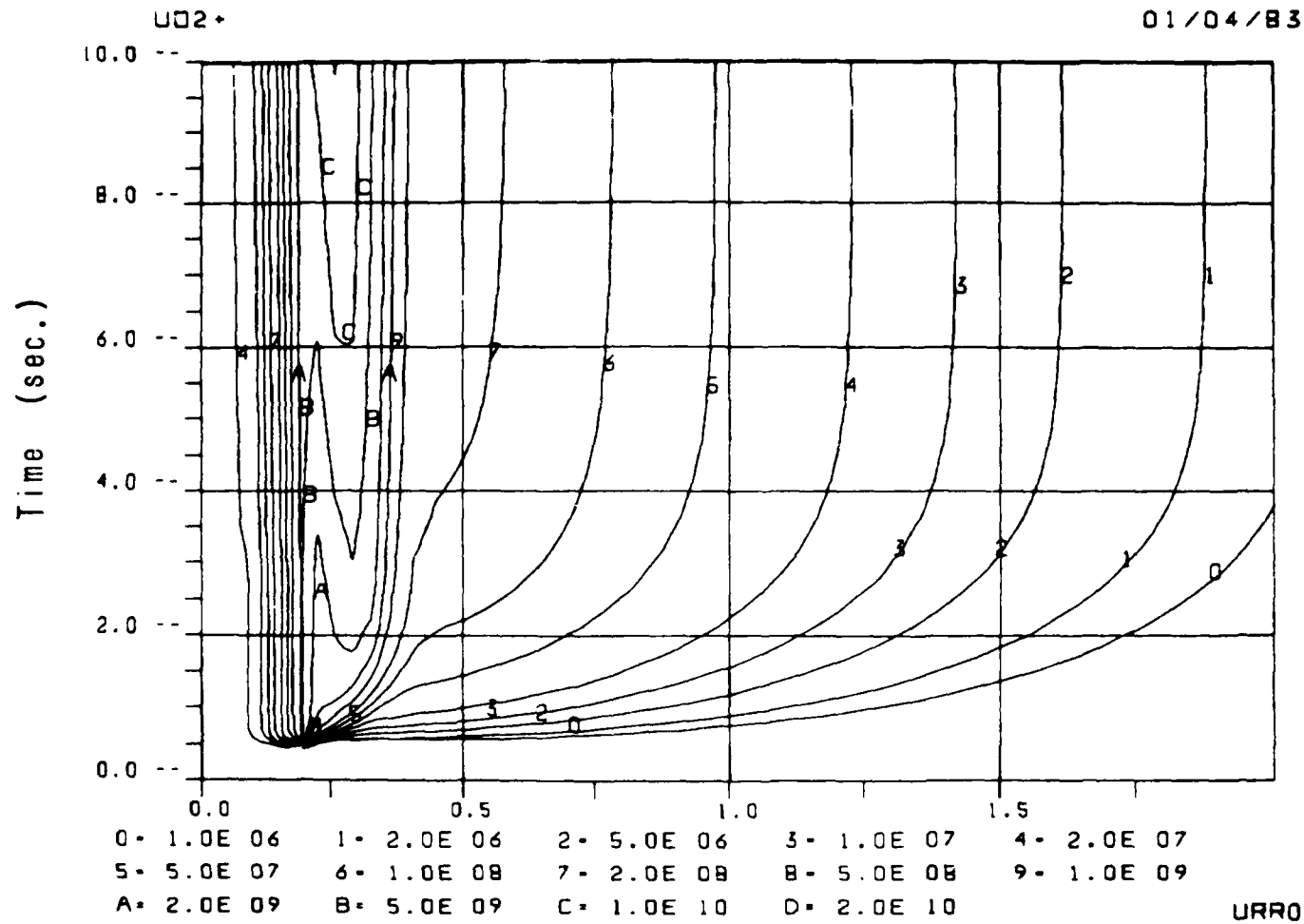

Figure 13. UO_2^+ ion concentration contours. Notice shell which forms gradually in time as UO^+ is oxidized by O_2 at about 0.25 km from release point.

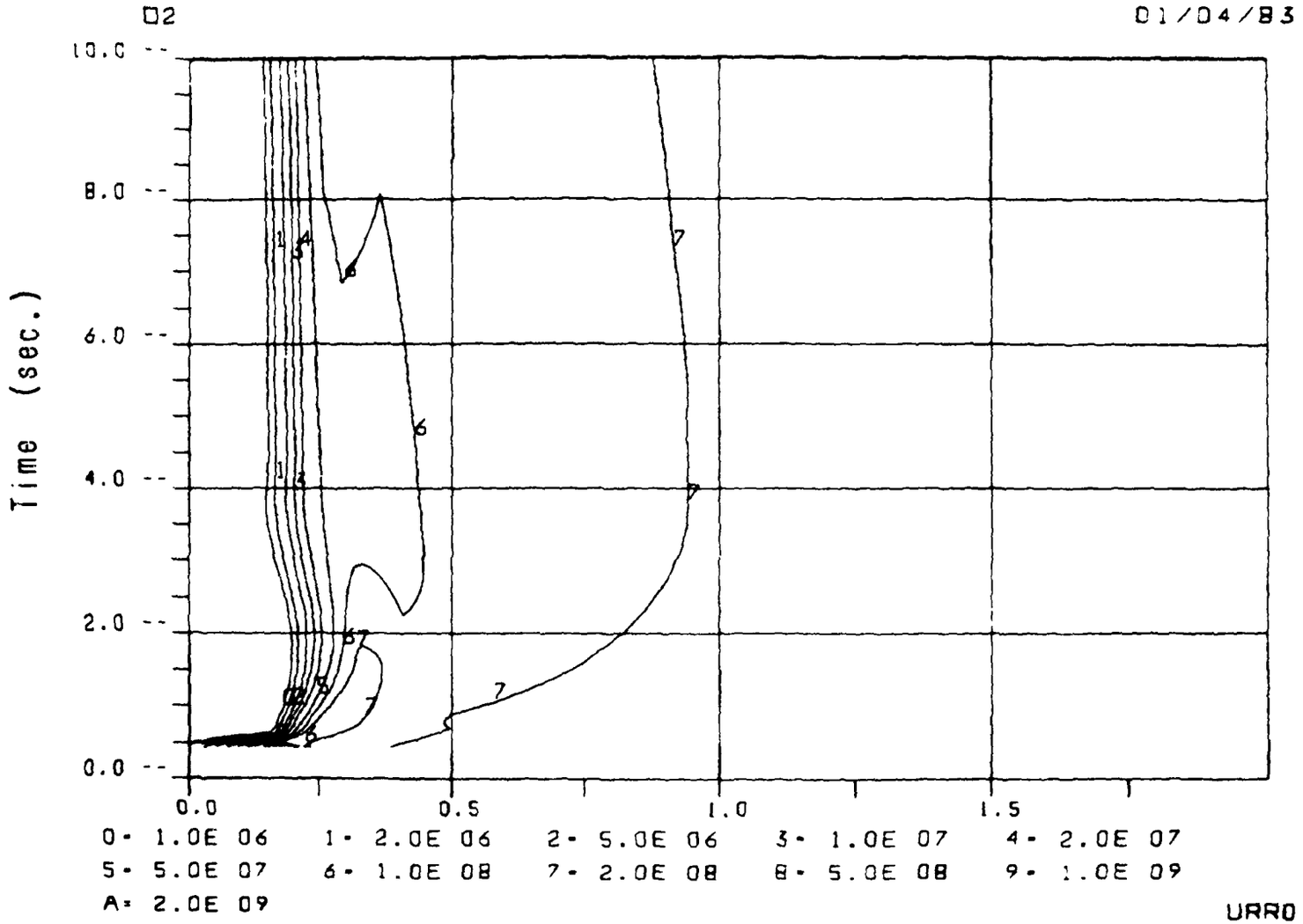

Figure 14. O_2 gas concentration contours. Notice deep hole created in O_2 near the release point which is only able to refill very slowly.

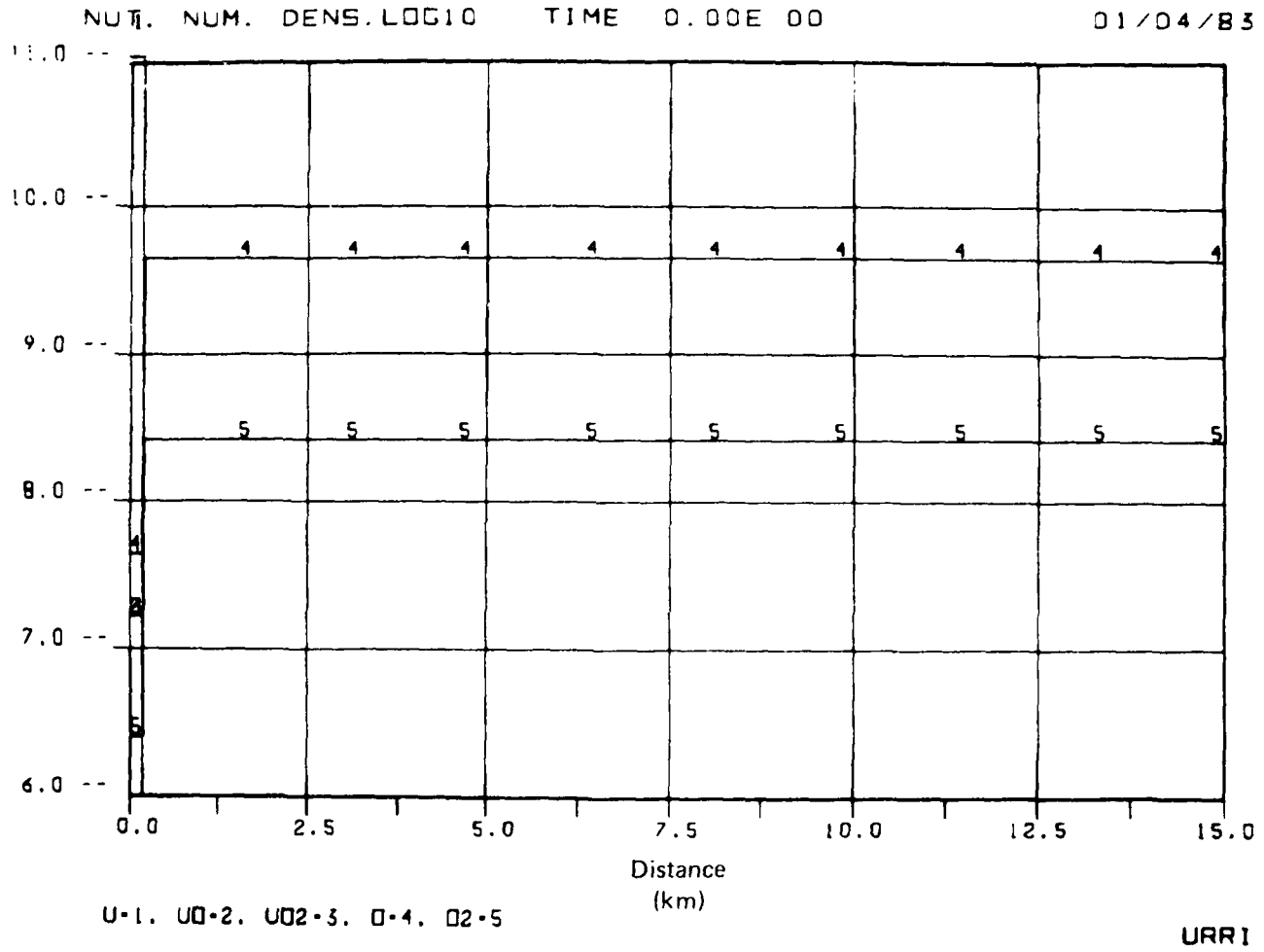

Figure 15. Initial conditions for simulation parallel to geomagnetic field and nominal diffusion. Same species are shown as in Fig. 1. Note the greatly expanded horizontal scale from Fig. 1.

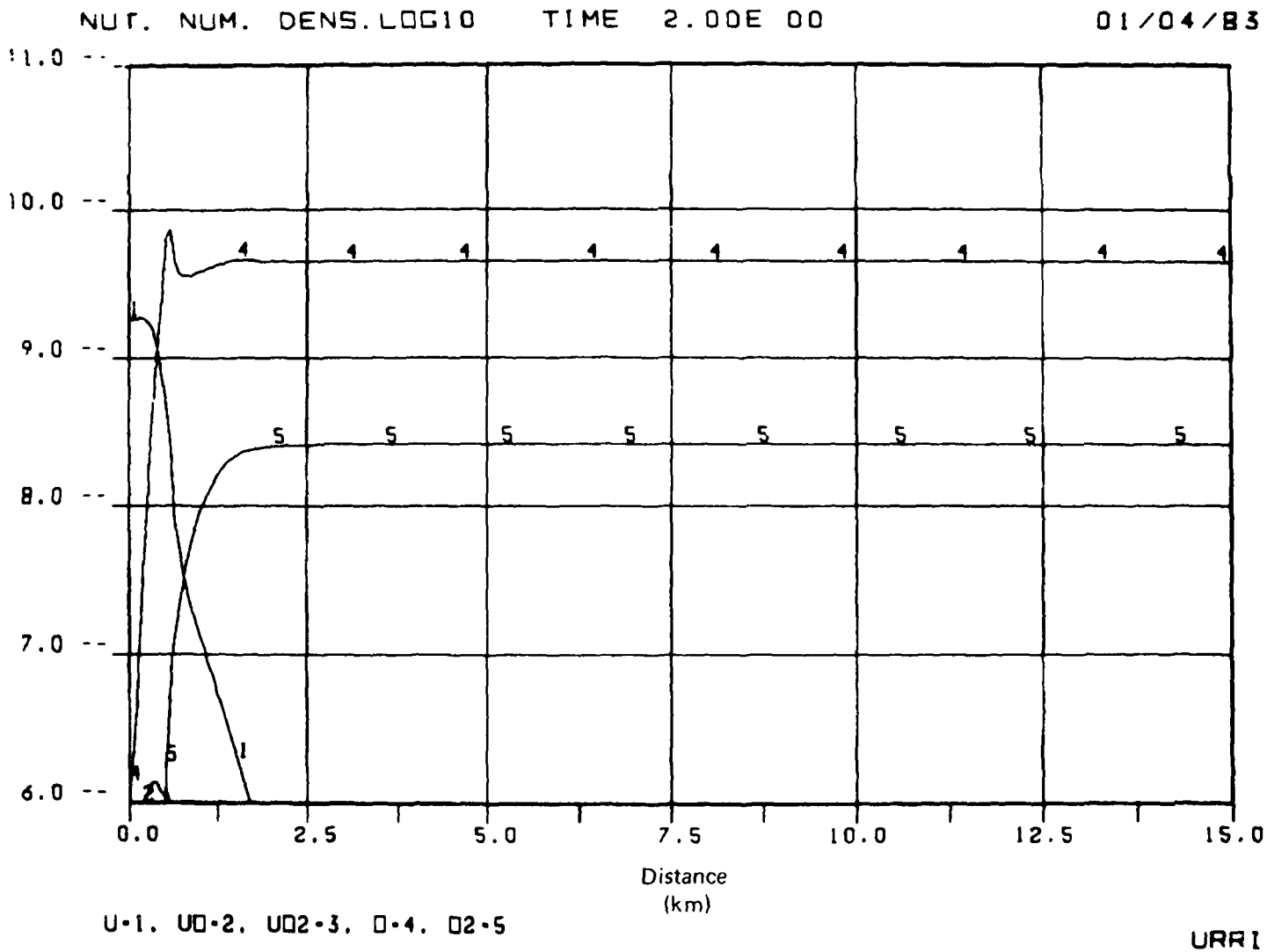

Figure 16. Neutral gas concentrations at 2 seconds after release.

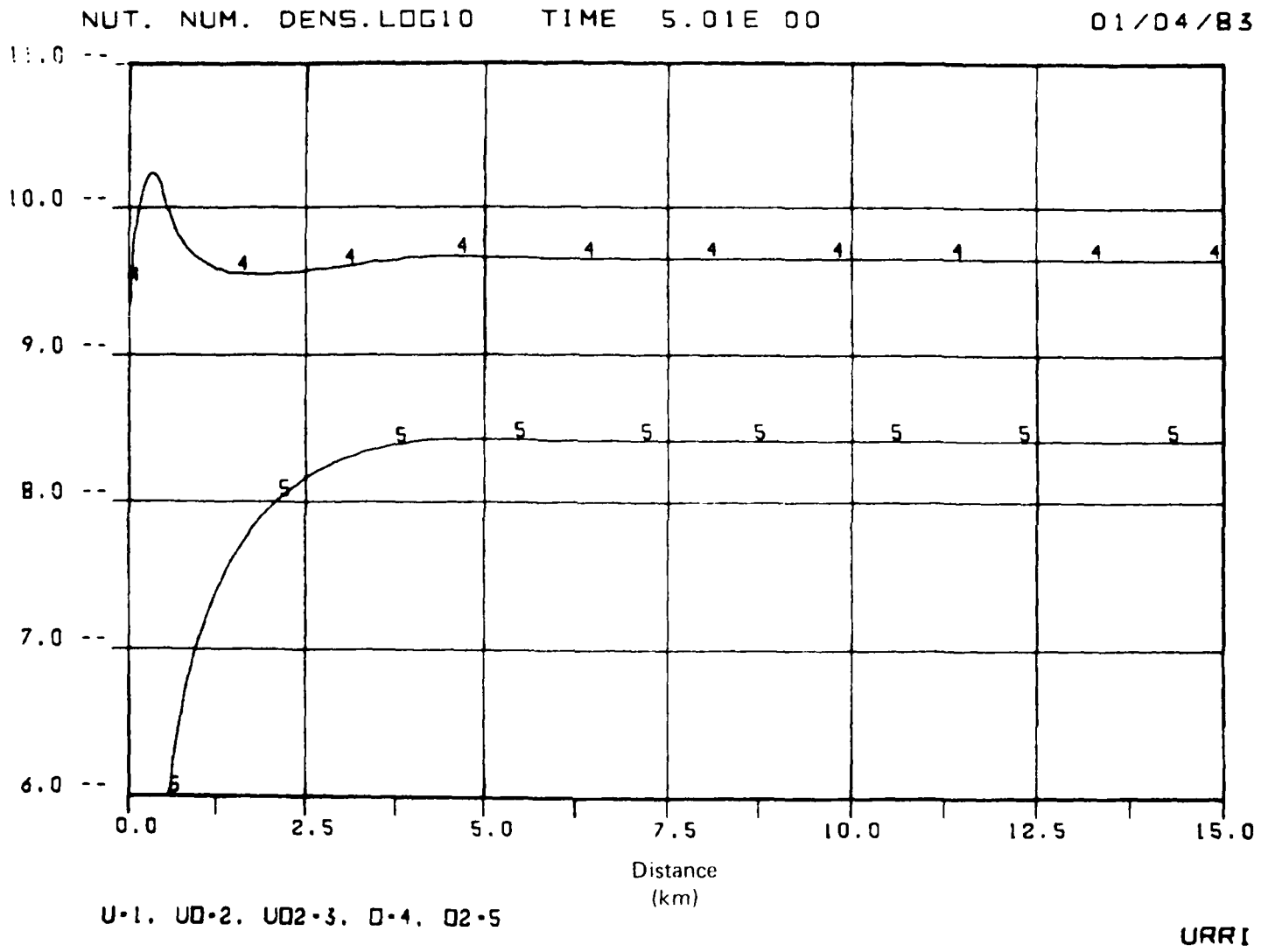

Figure 17. Neutral gas concentrations at 5 seconds after release.

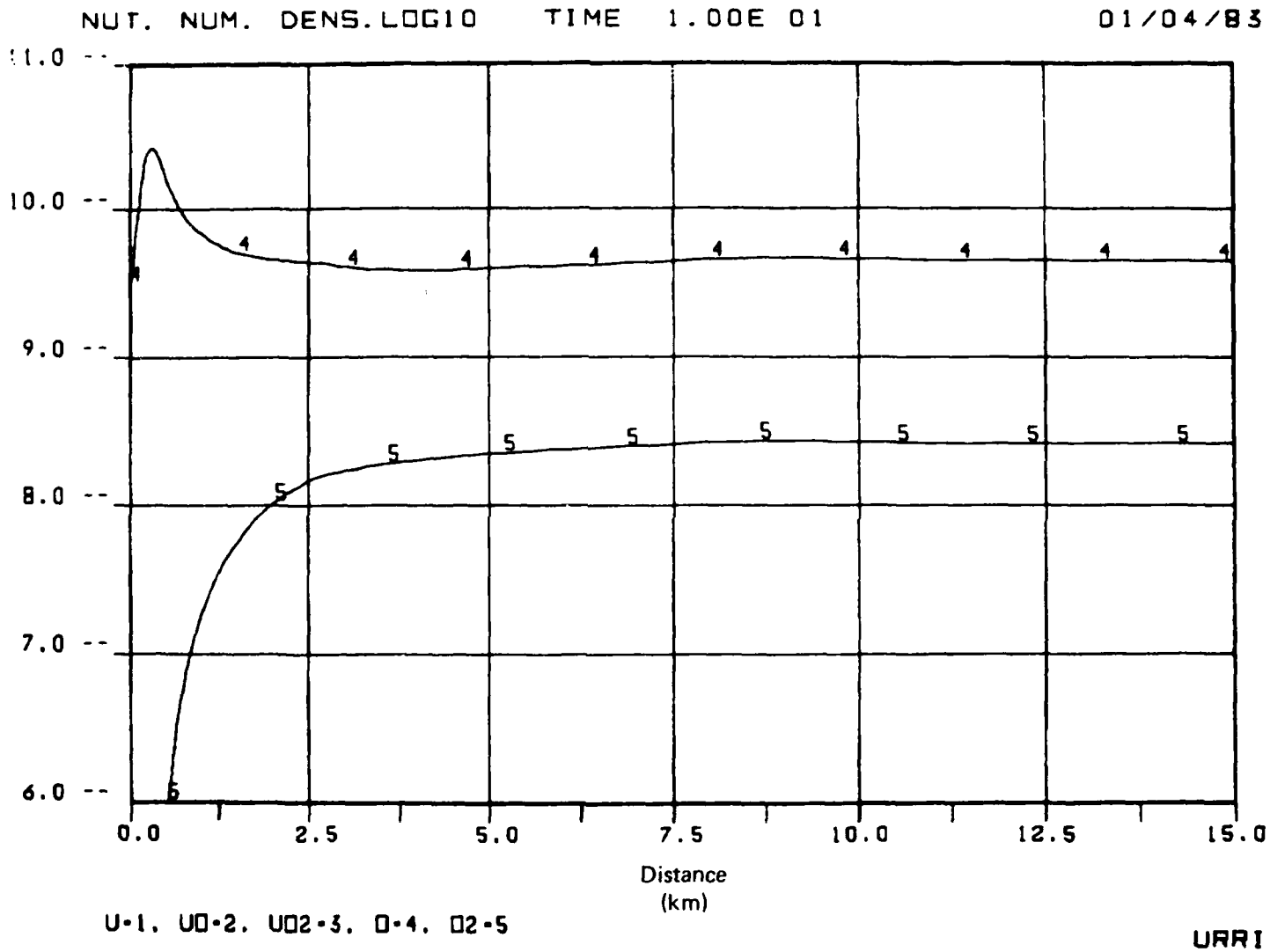

Figure 18. Neutral gas concentrations at 10 seconds after release.

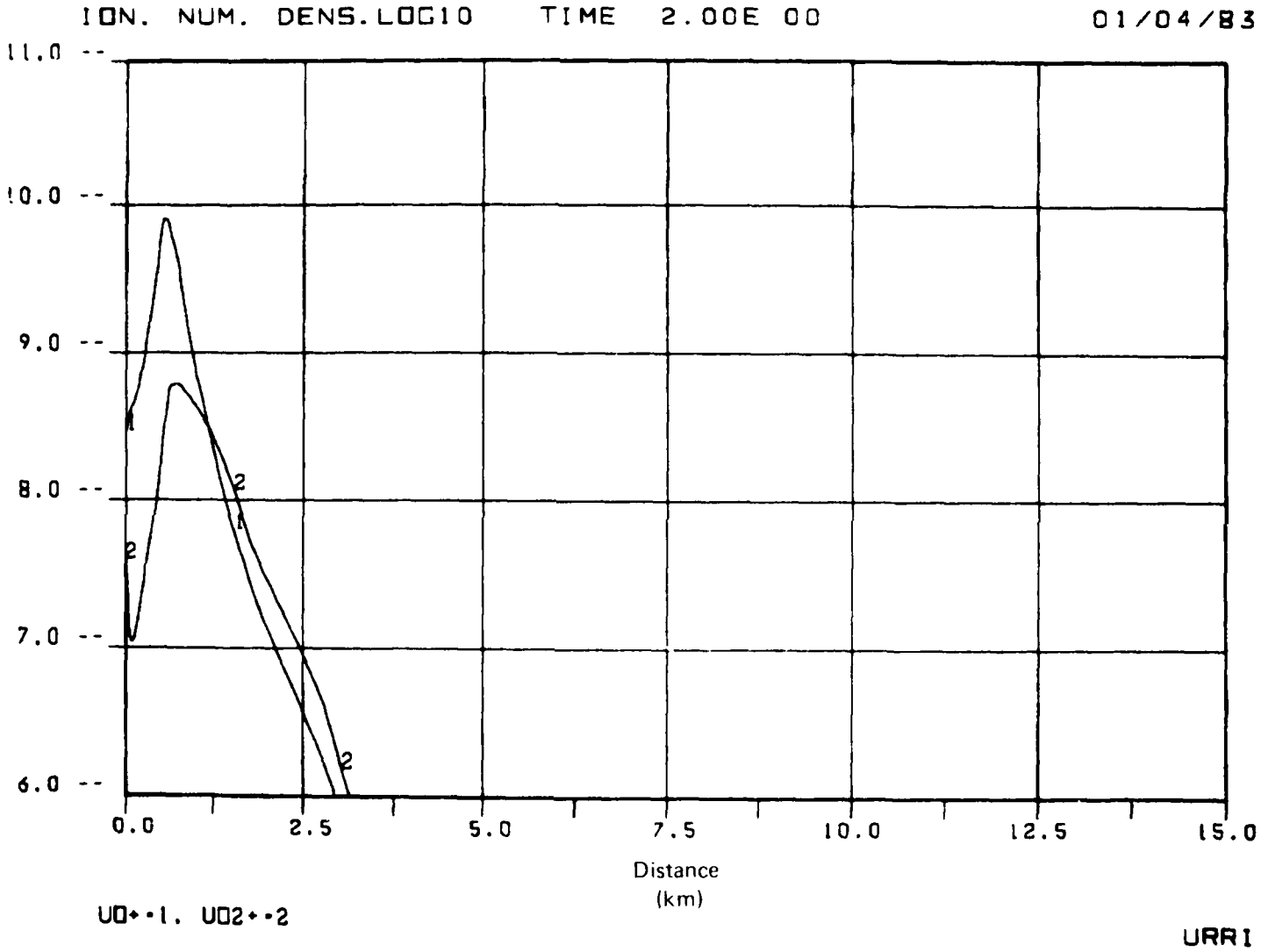

Figure 19. Ion concentrations for parallel simulation at 2 seconds, after release. Same species are shown as in Fig. 5.

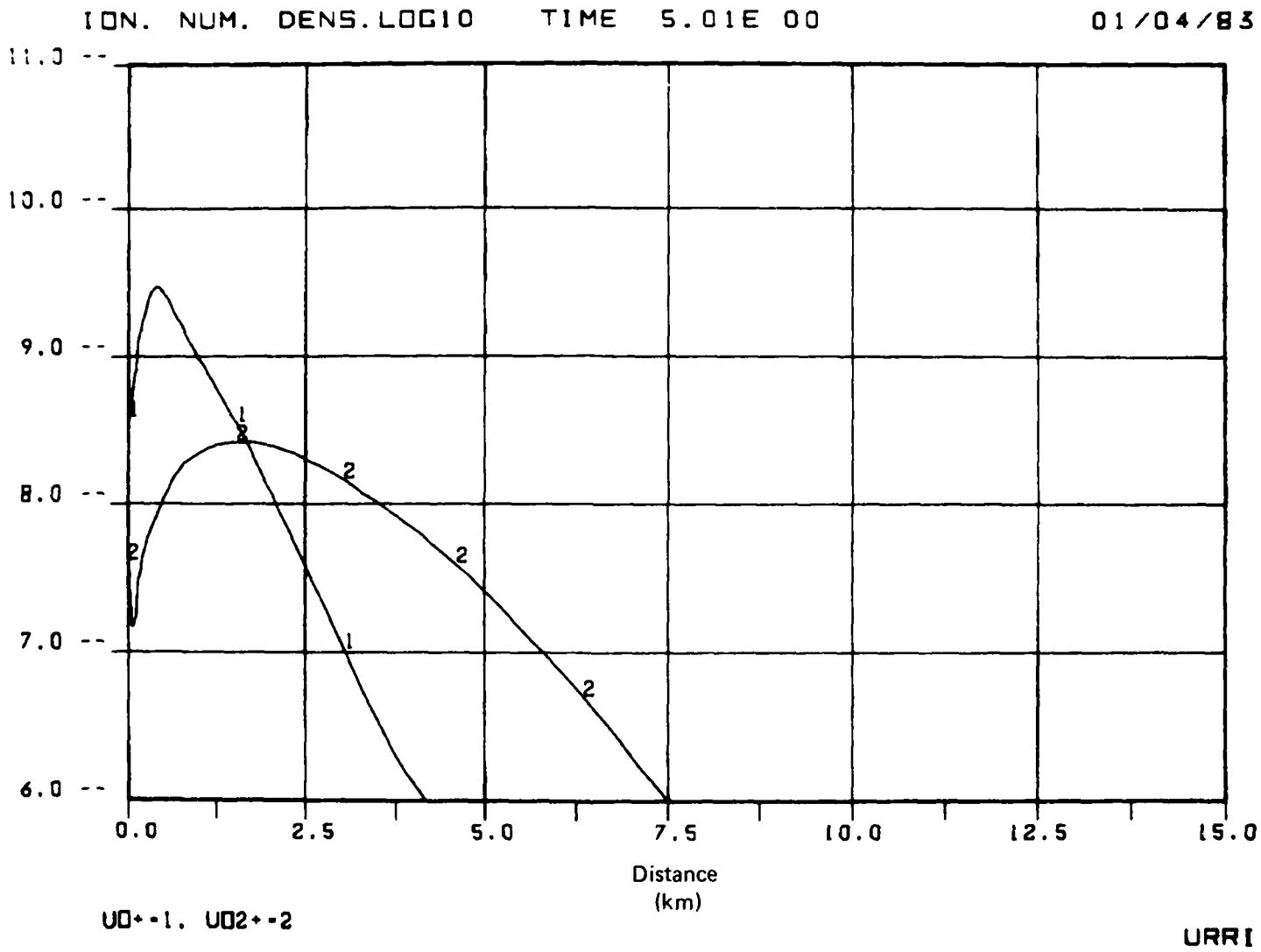

Figure 20. Ion concentrations at 5 seconds after release.

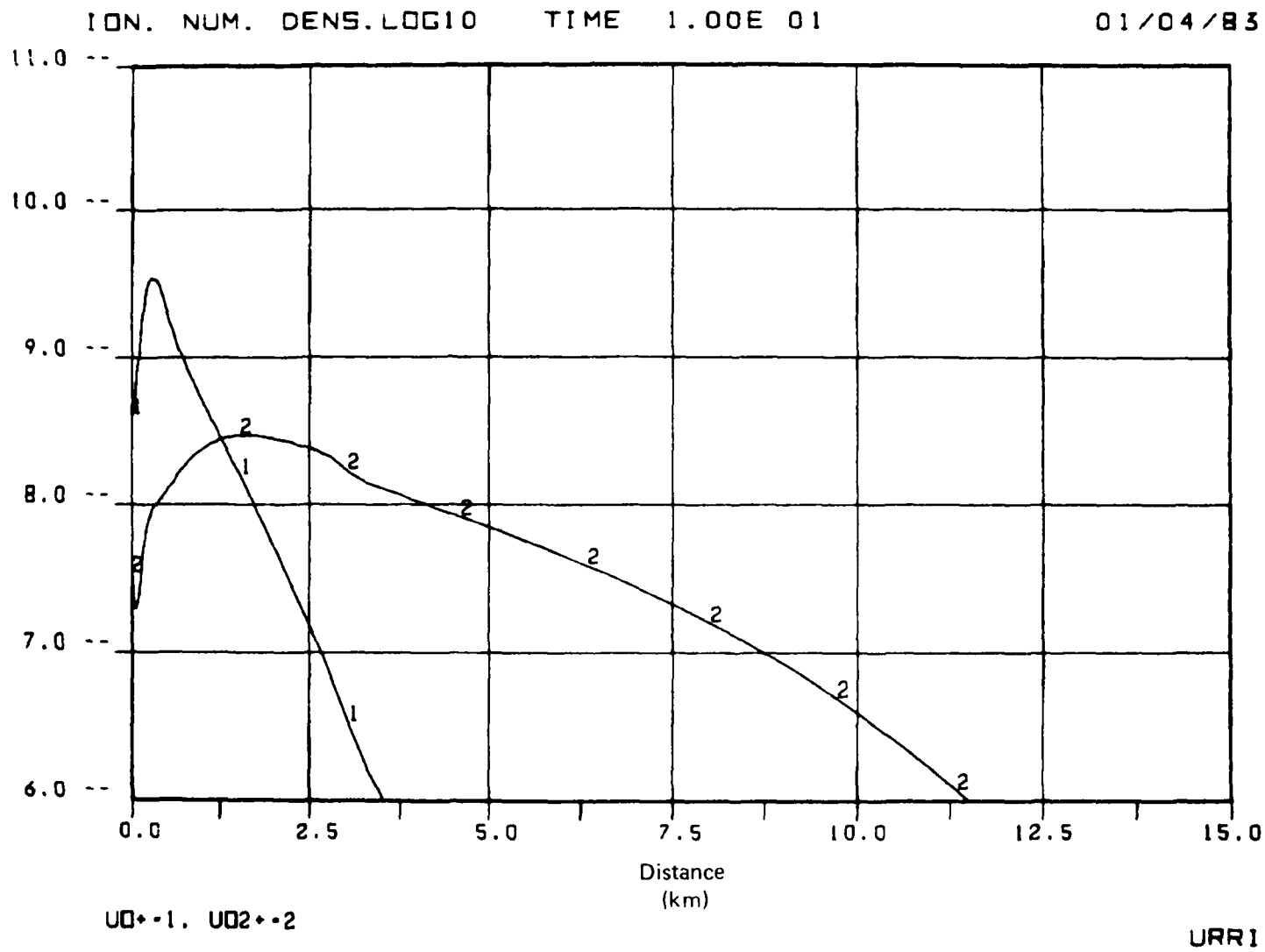

Figure 21. Ion concentration at 10 seconds after release.

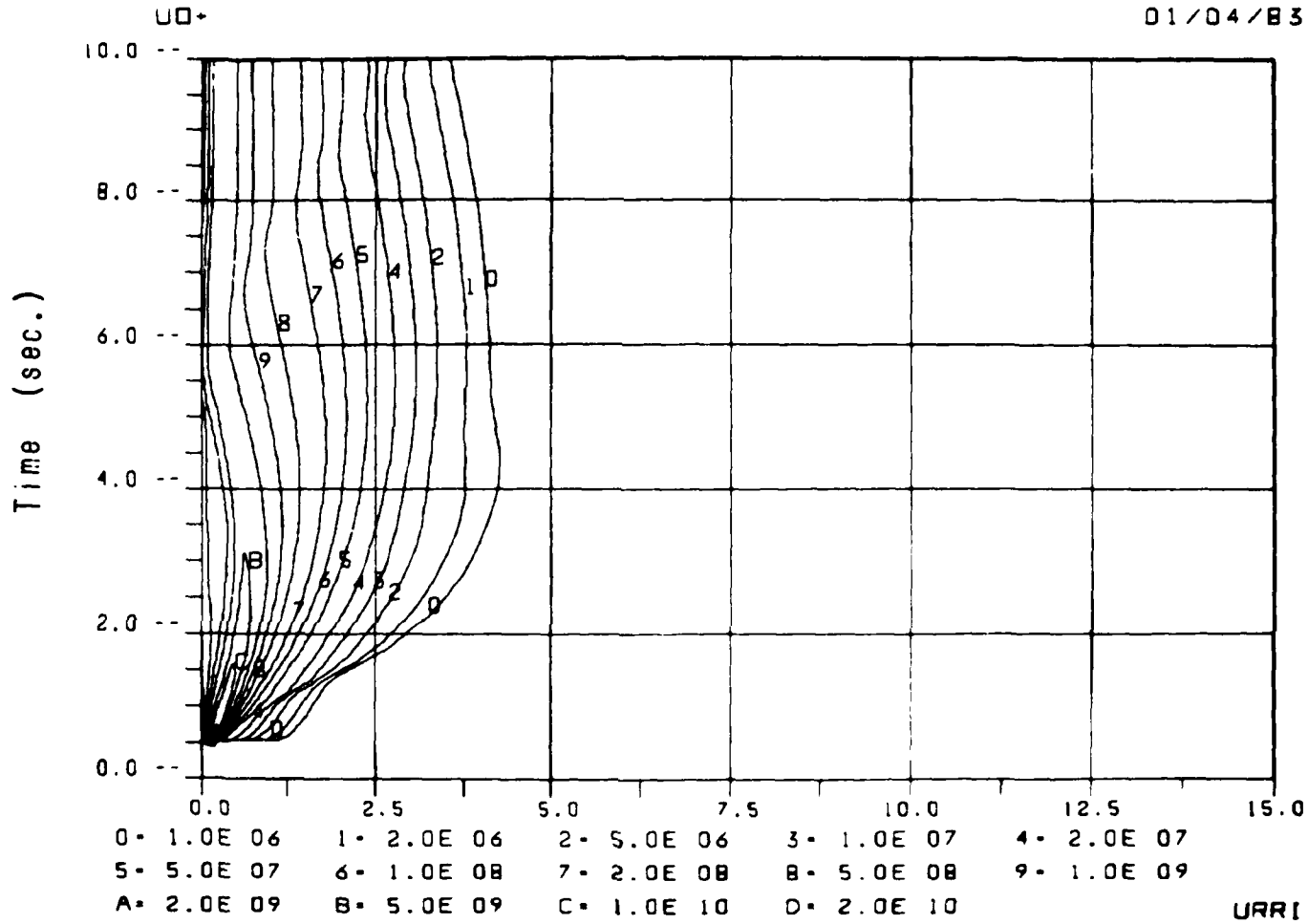

Figure 22. UO^+ concentration contours versus time and distance from release point for simulation parallel to geomagnetic field. Contours are in cm^{-3}. Notice shell formation at about 0.5 km from release point which is slowly consumed by oxidation to UO_2^+.

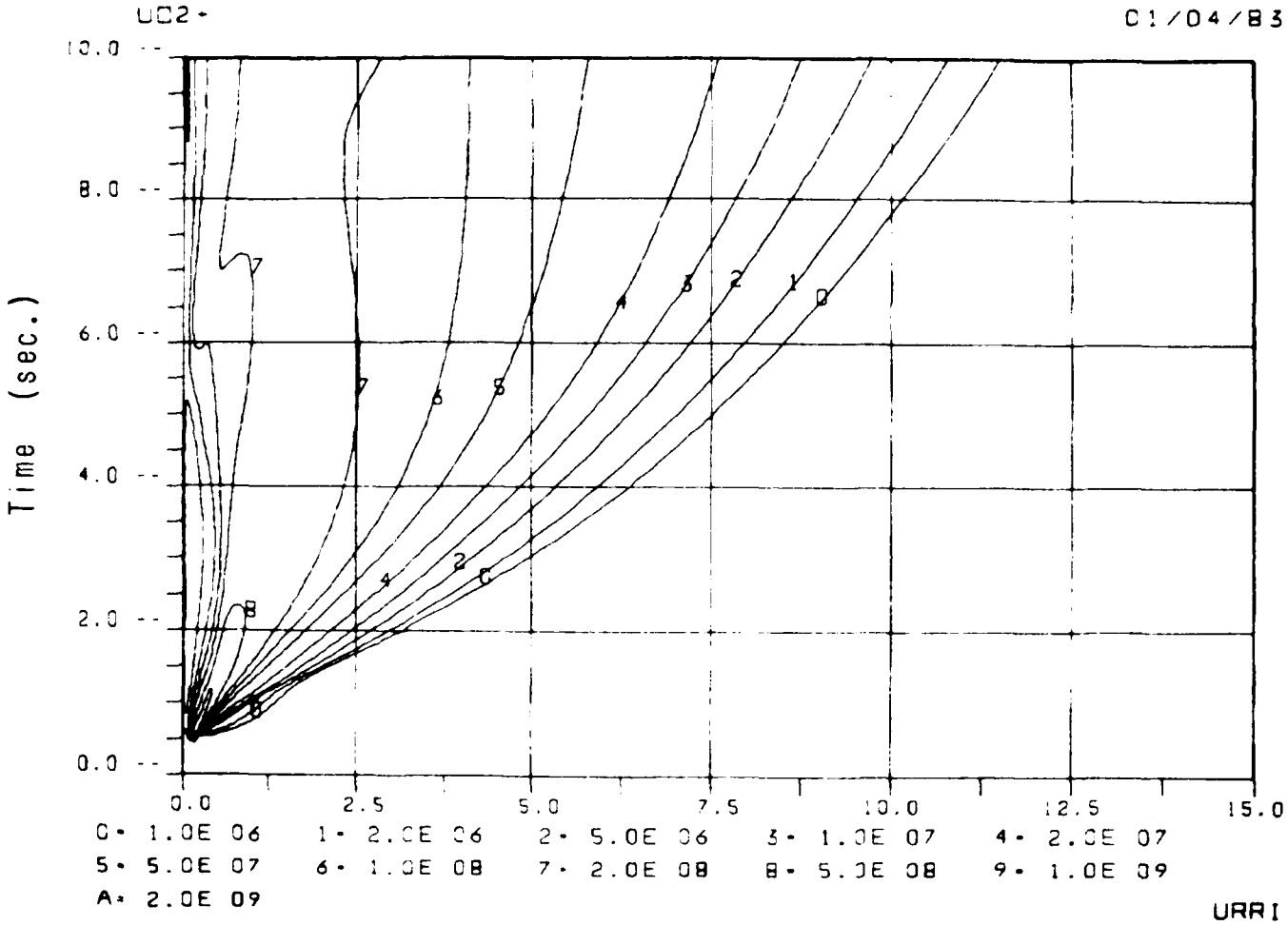

Figure 23. UO_2^+ concentration contours. Shell formation again takes place near release point, but in this case it spreads outwards owing to the action of nominal diffusion.

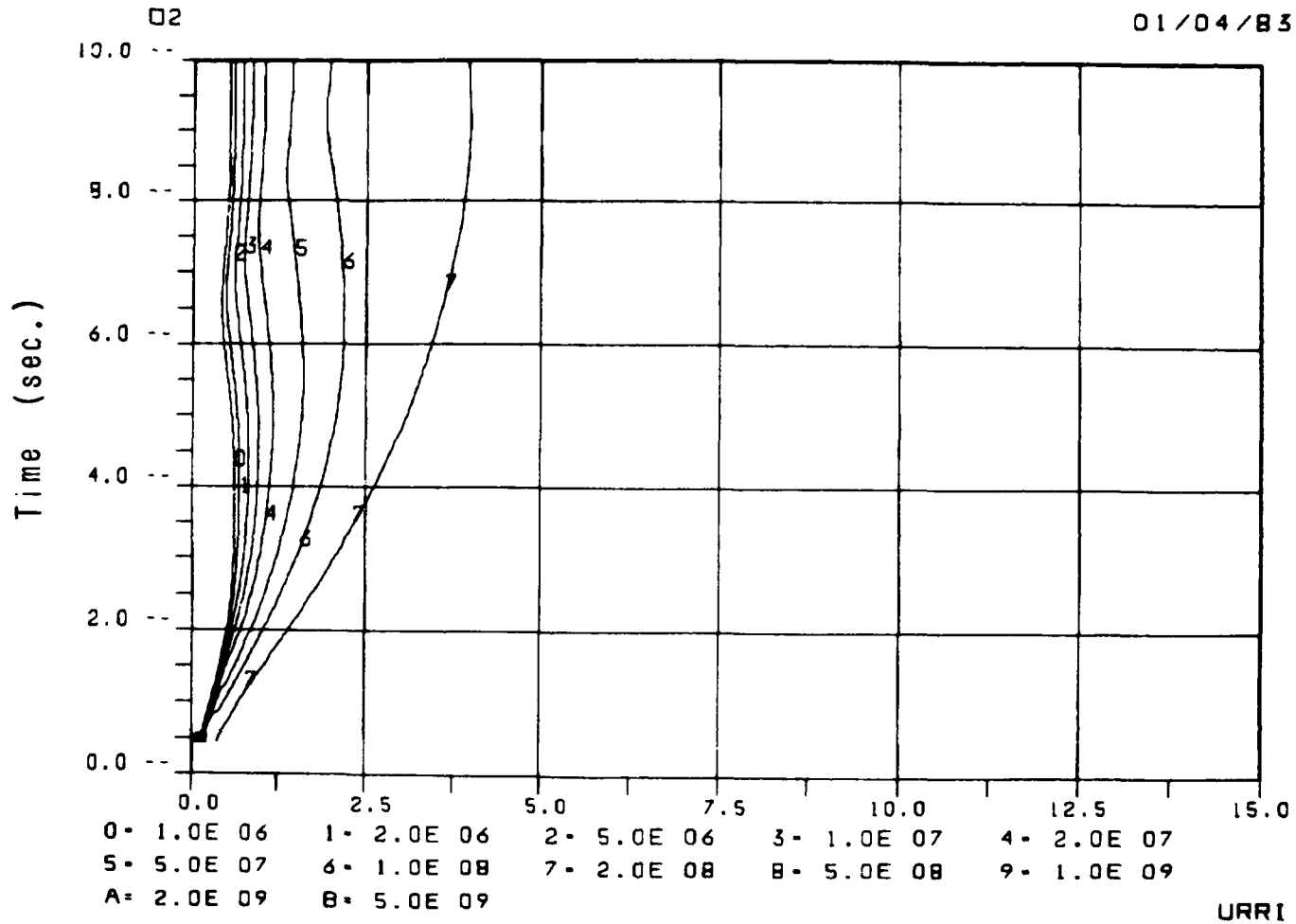

Figure 24. O_2 concentration contours. Note again the deep hole in O_2 formed in vicinity of release which only gradually refills after oxidation of U and UO^+ ceases.

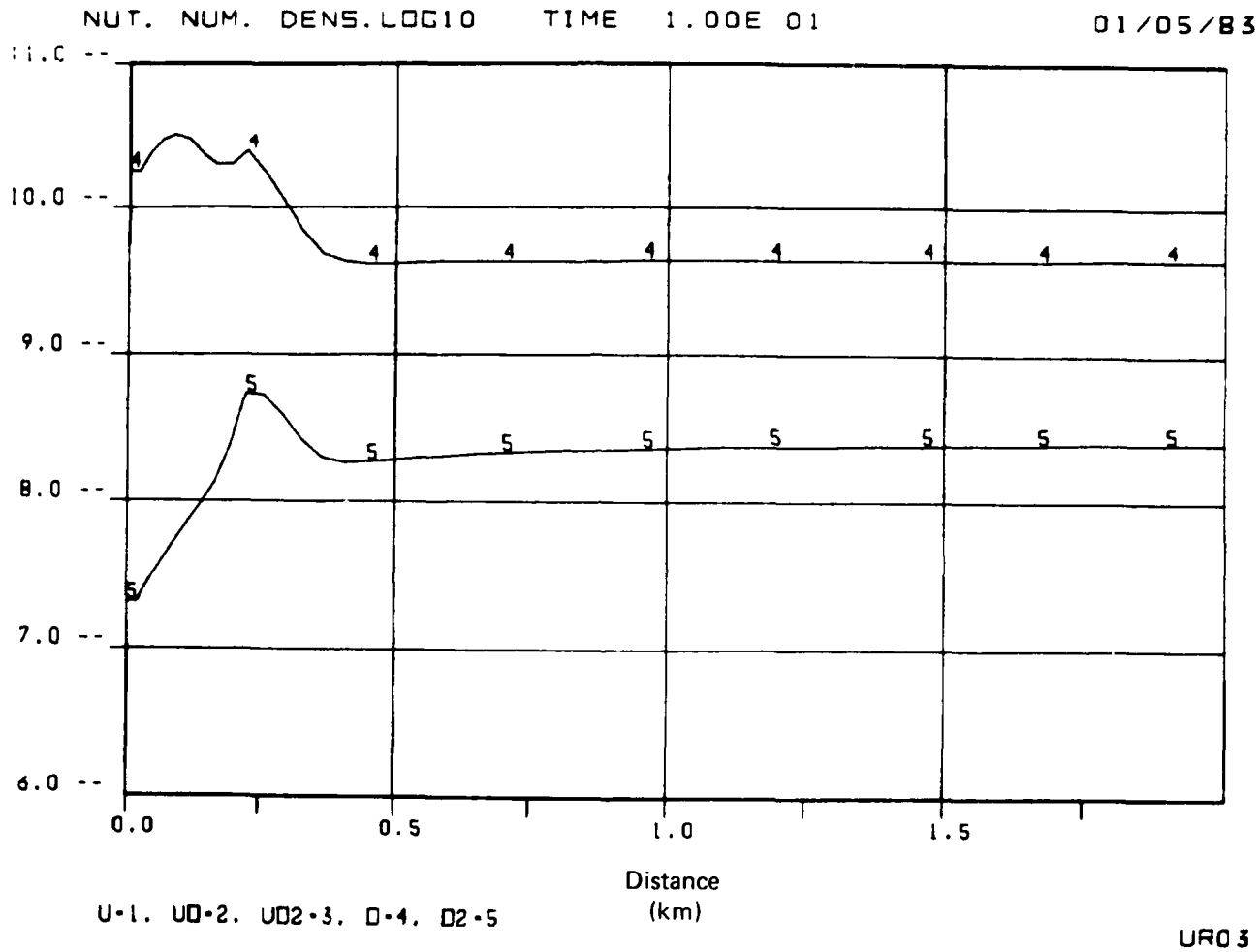

Figure 25. Neutral gas concentrations at 10 seconds for simulation perpendicular to geomagnetic field and faster than nominal diffusion.

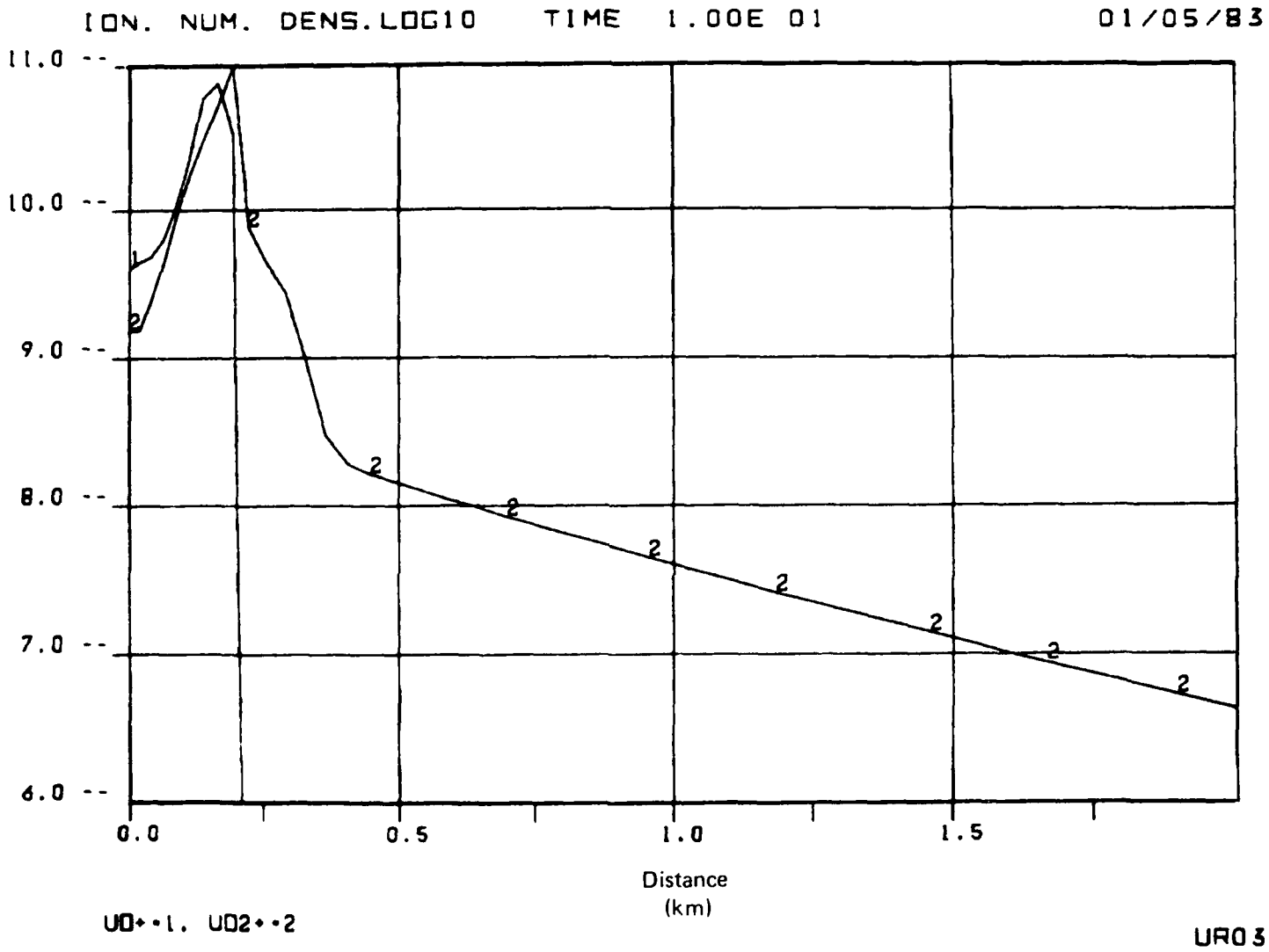

Figure 26. Ion gas concentrations at 10 seconds for simulation perpendicular to geomagnetic field and faster diffusion.

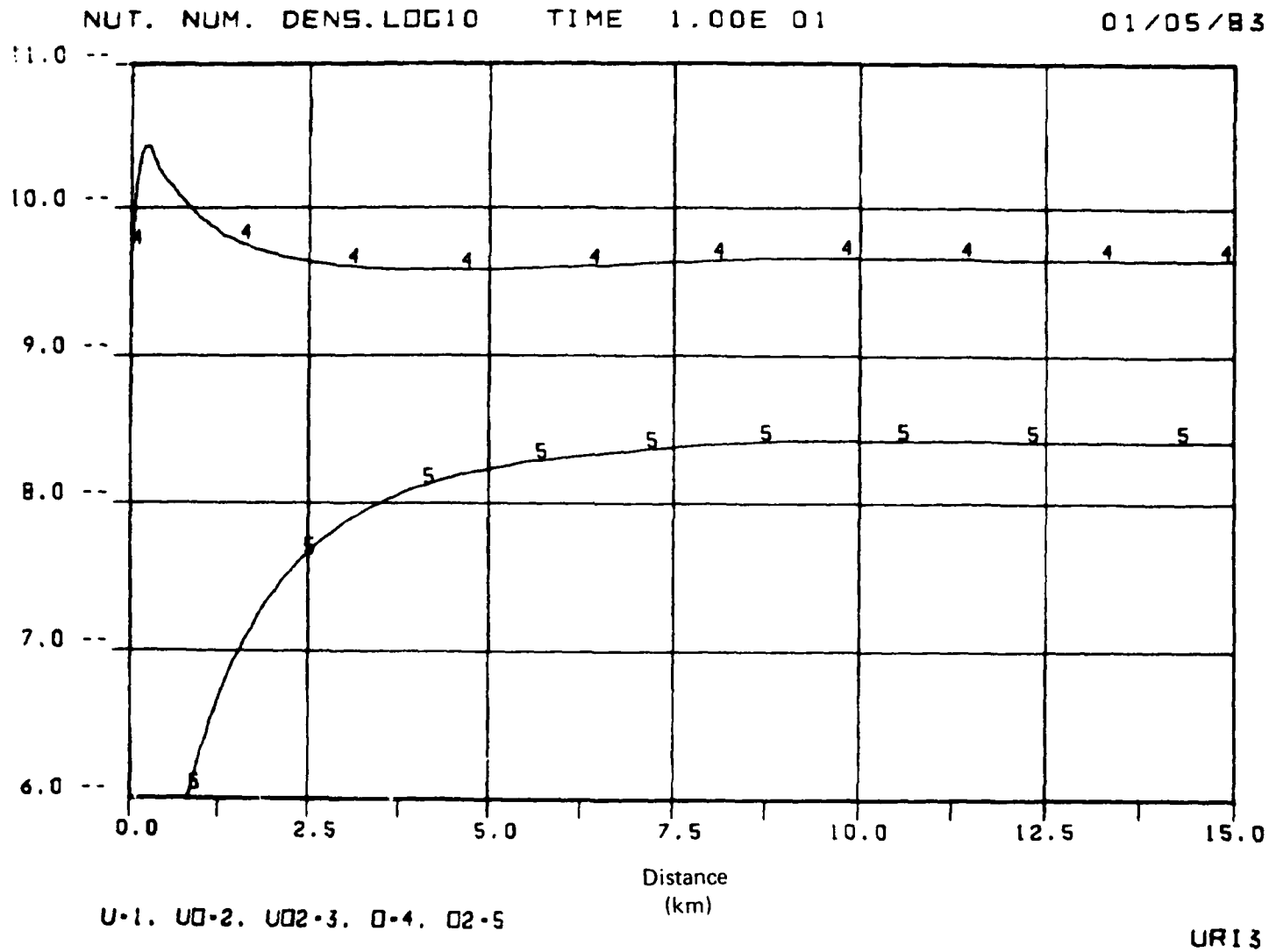

Figure 27. Neutral gas concentrations at 10 seconds for simulation parallel to geomagnetic field and faster diffusion.

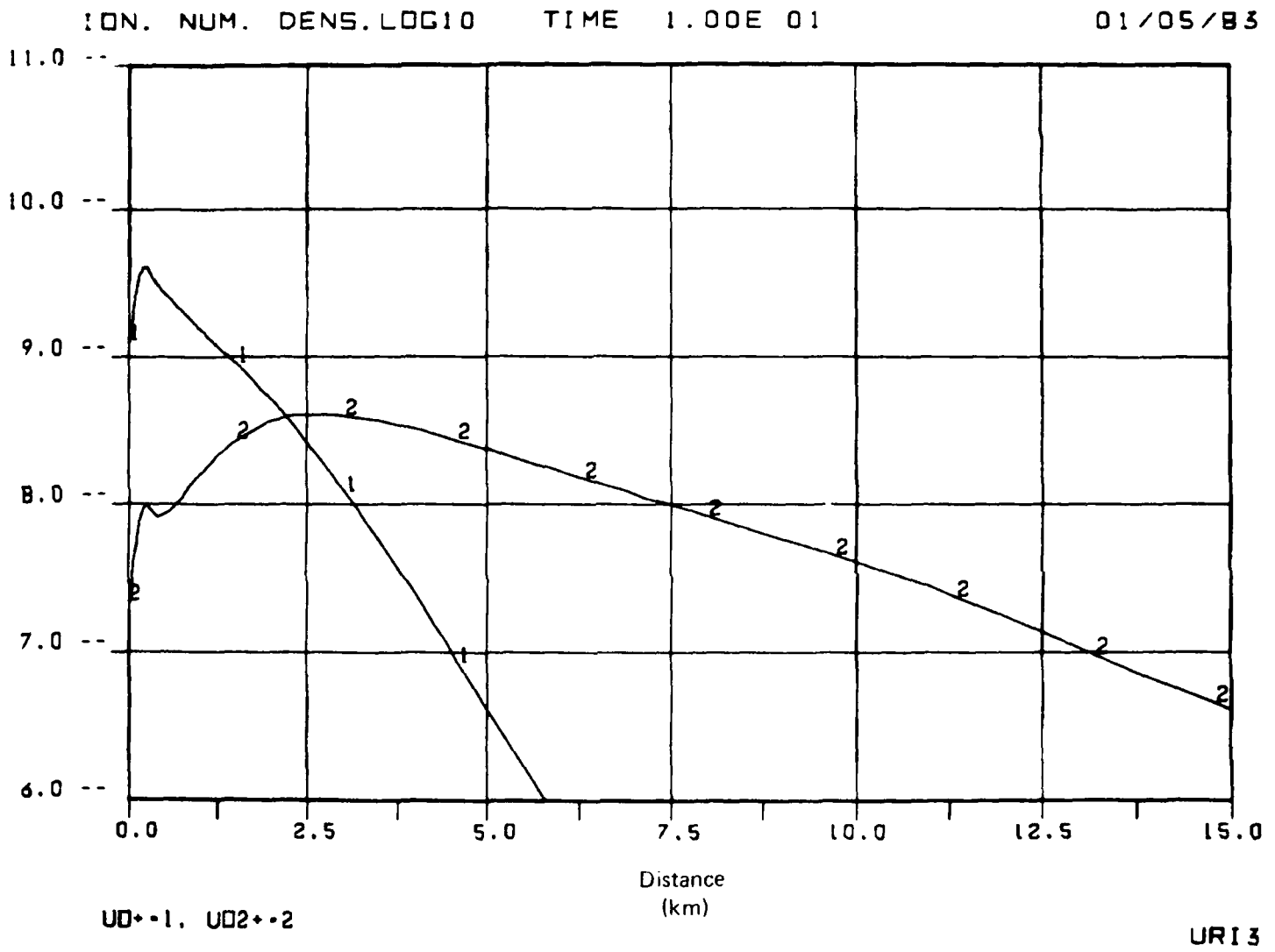

Figure 28. Ion gas concentrations at 10 seconds for simulation parallel to geomagnetic field and faster diffusion.

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