NACA TN 4321 10663

TECH LIBRARY KAFB, NM
0067278

NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS

TECHNICAL NOTE 4321

AN ANALYTICAL STUDY OF TURBULENT AND MOLECULAR MIXING IN ROCKET COMBUSTION

By David A. Bittker

Lewis Flight Propulsion Laboratory
Cleveland, Ohio

Washington
September 1958

AFMDC
TECHNICAL LIBRARY
AFL 2811

TECH LIBRARY KAFB, NM

0067278

NATIONAL ADVISORY COMMITTEE FOR AERONAUTICS

TECHNICAL NOTE 4321

AN ANALYTICAL STUDY OF TURBULENT AND MOLECULAR MIXING IN ROCKET COMBUSTION

By David A. Bittker

4834

CH-1

SUMMARY

An analytical study has been made to obtain an idea of the lengths needed for gaseous mixing in rocket combustion. Simplified models were assumed in which one gaseous propellant diffuses from several point sources into a uniform stream of the second gaseous propellant. No effects of the combustion process were considered in these models. Degrees of mixing were calculated at several positions downstream by assuming homogeneous turbulence in the main stream.

Detailed calculations were made for two different models. One assumes all the sources to be distributed in a single injection face. The other assumes sources distributed up to 7 inches downstream to simulate vaporization downstream of the initial injection point.

For the first model good mixing is achieved for all the assumed turbulence conditions at a low ratio of downstream distance to source spacing; the estimated mixing lengths are less than lengths required for evaporation of typical rocket-engine sprays. Proper mixing takes significantly longer for the downstream sources model.

Calculations show that the contribution of molecular diffusion to the over-all mixing is negligible in these simple models, and mixing is therefore controlled entirely by the turbulence parameters. This fact makes the obtained results independent of any particular propellant combination.

These approximate calculations indicate that gaseous mixing generally occurs faster than spray evaporation. Its effect on the combustion rate certainly cannot be neglected, however, especially when sources are distributed downstream of the first injection point.

INTRODUCTION

The many physical processes which occur simultaneously in rocket combustion make the entire process extremely complex (ref. 1). The study of each process individually is one approach to identifying those that limit the rate of the combustion. The combustion chamber length required for evaporation of liquid-propellant sprays has already been studied (refs. 2, 3, and 4). The present work estimates the combustion-chamber lengths required to mix propellants by turbulent and molecular gaseous-diffusion processes.

A model and theory have been developed for calculation of gas concentration profiles for systems in which both propellant vaporization and gaseous diffusion occur (ref. 5, p. 76). To satisfy the purposes of this preliminary survey, the complete treatment of reference 5 has not been used. Instead calculations for turbulent and molecular diffusion of gases have been carried out for simplified analytical models. The results are then compared with those from the vaporization calculations.

SYMBOLS

C	concentration of diffusing gas, lb/cu ft
D	turbulent diffusion coefficient, sq ft/sec
d	molecular diffusion coefficient, sq ft/sec
L	scale of turbulence, ft
p	ambient pressure, lb/sq in. abs
r	radial distance in a y-z plane from any point in the stream to the axial line through a source
s	source spacing in the y-z plane, in.
T	turbulence intensity, $\sqrt{\overline{u^2}}/U$
U	constant mean stream velocity, ft/sec
$\sqrt{\overline{u^2}}$	root-mean-square turbulent-velocity fluctuation in any direction
W	source strength, lb/sec
x	distance downstream of injection plane

α $T(x/s)$

σ_g standard geometric deviation

ψ ripple factor

ω spreading factor, sq ft

Subscripts:

max maximum

min minimum

4834

CI-1 back

THEORY AND MODELS FOR THE CALCULATIONS

General Theoretical Equations

The differential equation for combined molecular and turbulent mass transfer in three dimensions is (ref. 5, p. 63):

$$\frac{\partial C}{\partial \omega} = \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \tag{1}$$

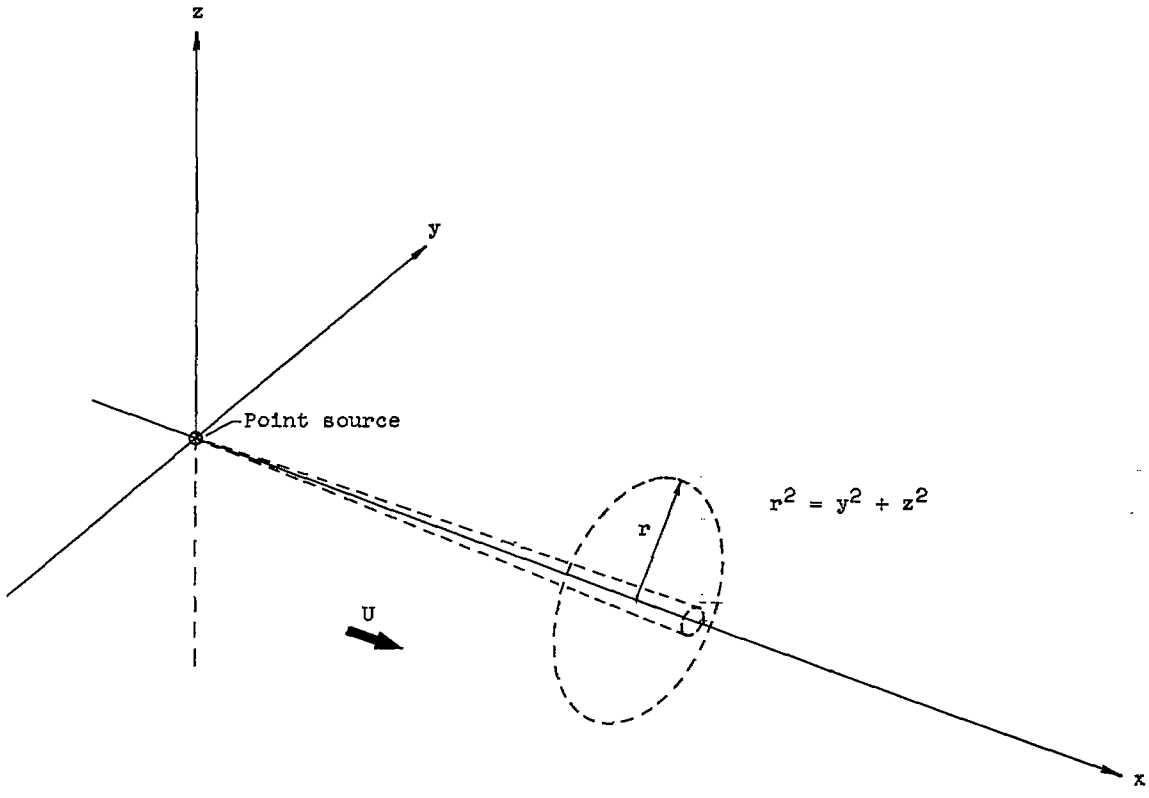
where C is the concentration of the diffusing substance at a given position and time, and ω, the time-dependent spreading coefficient, is defined by

$$\omega = \int_0^t (D + d)\, dt' \tag{2}$$

In the models to be described later all diffusion is assumed to come from a number of continuous point sources. Each point source is assumed to contribute independently to the total concentration of the diffusing gas at any given point. A good approximate solution of equation (1) for a continuous point source is given in reference 5 as

$$\frac{C}{W/U} = \frac{1}{4\pi\omega} e^{-r^2/4\omega} \tag{3}$$

This equation pertains to the diffusion model shown in the following sketch:



Material diffuses into an infinite stream of uniform density flowing in the x-direction with linear velocity U. The equation involves three assumptions: (1) the source material occupies negligible volume in the main stream, (2) diffusion in the x-direction is negligible, and (3) r is very much smaller than x. In connection with the last assumption, however, inspection of the data of reference 6 (p. 16) indicates that the error involved in using this equation at r/x values up to 0.4 is negligible for the purposes of this report. The spreading factor ω is evaluated at time $t = x/U$. A simple analytical expression for ω obtained under the assumption of homogeneous turbulence is (ref. 5, p. 63)

$$\omega = LxT + L^2(e^{-xT/L} - 1) + \frac{xd}{U} \tag{4}$$

where L is the scale of the turbulence and T is the turbulence intensity, defined as the ratio of the root-mean-square velocity fluctuation to the mean stream velocity.

It should be noted that the concentration C in equation (3) is a time average value and tells nothing about the fluctuation of concentration with time at any point. It should also be noted that the effect on mixing of the combustion process is not being considered in these equations.

For diffusion from a number of point sources, mixing at any point can most readily be shown in terms of a "ripple factor." This factor is defined as

$$\psi = \frac{C_{min}}{C_{max}} \tag{5}$$

The terms C_{min} and C_{max} are the lowest and highest values of the diffusing-material concentration at the particular downstream distance. The ripple factor for perfect mixing is unity.

It can be pointed out here that perfect mixing is unnecessary for complete combustion except at stoichiometric propellant ratios. Mixing in a combustion process has to proceed only to a point where one propellant has been completely consumed. However, a high degree of mixing is important in achieving a uniform temperature profile in the hot gases, and thus, high performance.

Models Used

Two models were used in these calculations. They are illustrated in figures 1 and 2 in which some typical concentration profiles are shown qualitatively. These models are as follows:

Model 1: An infinite rectangular grid of equal strength, evenly spaced point sources in the $x = 0$ plane.

Model 2: A lattice made up of eight grids of sources as described for model 1. The grids are spaced at 1-inch intervals downstream along the axis of flow with the first one at the $x = 0$ plane.

The time-average diffusing substance concentration at any point is assumed to be the sum of contributions from all sources acting independently at that point, so that equation (3) can be used. The results apply only for the situation where no burning takes place and where the diffusing-material volume is small compared with the mainstream volume. All calculations performed with these models neglect any boundary effects. (These wall effects can be calculated using the theory of ref. 7.)

METHOD OF CALCULATION

Assignment of Turbulence Parameters

The calculation of downstream concentration profiles using the preceeding equations requires numbers for the turbulence scale and intensity. Here a temporary impasse appears, inasmuch as these values are not known

for the rocket-combustion environment. Preliminary calculations showed that turbulent mixing is not affected by the scale (the over-all size of the eddies) except at very small values. Therefore, a scale value of 0.1 foot, based on pipe-turbulence data, was arbitrarily used throughout these calculations. A series of turbulence-intensity values was used. The intensities used, and also the downstream distances and source spacings (in the $x = 0$ plane), are as follows:

$$T = 0.05,\ 0.07,\ 0.09,\ 0.11$$

$$x = 1 \text{ to } 12 \text{ in. at intervals of } 1/2 \text{ or } 1 \text{ in.}$$

$$s = 1/2 \text{ and also } 1 \text{ in. for model 1 only}$$

4834

Relative Contributions of Molecular and Turbulent Diffusion

At this point it is possible to evaluate the relative contributions of turbulent and molecular diffusion to the entire mixing process by calculating the two separate contributions to the spreading factor ω. This task requires using a particular propellant combination and assuming specific flow conditions. The system oxygen diffusing into hydrogen has been used, because this combination has the largest molecular diffusion coefficient at any given temperature and pressure. Furthermore, to exaggerate the contribution of the molecular diffusion term to the spreading factor ω, low values of turbulence level were assumed as follows:

Scale of turbulence, L, ft	0.10
Turbulence intensity (normal pipe flow value), T	0.03
Ambient pressure, p, lb/sq in. abs	600
Constant mean stream velocity, u, ft/sec	100
Average molecular-diffusion temperature, °R	400

The molecular-diffusion coefficient for these conditions is 1.207×10^{-5} square feet per second as calculated by the equation of reference 8. The result of this calculation shows that the maximum contribution of the molecular diffusion term to the whole spreading factor is only 0.3 percent of the turbulent-mixing contribution under the assumed conditions. It can be concluded that molecular diffusion is always negligible for the models employed, regardless of the propellant combination chosen.

3834

Calculations Involving the Ripple Factor

Analytical expressions for the ripple factor can be obtained as a result of neglecting molecular diffusion. The general equation for the ripple factor for n continuous point sources is

$$\psi = \frac{C_{min}}{C_{max}} = \frac{a_1 e^{-r_1^2/4\omega} + a_2 e^{-r_2^2/4\omega} + \ldots a_n e^{-r_n^2/4\omega}}{b_1 e^{-(r_1')^2/4\omega} + b_2 e^{-(r_2')^2/4\omega} + \ldots b_n e^{-(r_n')^2/4\omega}} \tag{6}$$

where

r = r value for C_{min}

a = number of sources having a given value of r

r' = r value for C_{max}

b = number of sources having a given value of r'

The equation can be simplified in its application to model 1 by neglecting all but the most important source contributions. Details are given in the appendix for the derivation of an approximate equation for model 1. The final result and the assumptions used to obtain it are as follows:

Assumption 1: Only sources with $r = s\sqrt{2}/2$, $s\sqrt{10}/2$, and $s\sqrt{18}/2$ contribute to C_{min}.

Assumption 2: Only sources with $r' = 0$, s, and $s\sqrt{2}$ contribute to C_{max}.

The resulting equation is

$$\psi = \frac{4e^{-(1/4\alpha^2)} + 8\left[e^{-(1/4\alpha^2)}\right]^5 + 4\left[e^{-(1/4\alpha^2)}\right]^9}{1 + 4\left[e^{-(1/4\alpha^2)}\right]^2 + 4\left[e^{-(1/4\alpha^2)}\right]^4} \tag{7}$$

where $\alpha = T(x/s)$

RESULTS AND DISCUSSION

Model 1

Figures 3(a) and (b) show results of the detailed ripple-factor calculations for this grid of sources model. At the 1/2-inch source spacing (fig. 3(a)) the ripple factor becomes equal to 0.95 at an x value of 5.8 inches for the lowest turbulence intensity used ($T = 0.05$). This fact indicates that mixing due to turbulence is fairly rapid for a source spacing typical of injector port spacings in a rocket engine.

Mixing occurs much more slowly for the 1-inch spacing (fig. 3(b)). This difference in the degree of mixing is resolved in figure 4 where the ripple factor is plotted as a function of the ratio of downstream distance to source spacing. For a fixed turbulence intensity these plots show that the degree of mixing is a function of the ratio x/s, within an accuracy of 10 percent.

The dependence of ripple factor on turbulence intensity is shown in figure 5. Obviously mixing increases with increasing intensity.

Comparison with Approximate Equation

The approximate equation for ripple factor (eq. (7)) predicts that mixing is independent of turbulence scale for this model and depends only on the turbulence intensity and the ratio of downstream distance to source spacing (x/s). This equation is shown in the semilogarithmic plot of figure 6 with the curve for the detailed calculations. In these plots high values of $\alpha = T(x/s)$ give good mixing. The comparison shows that equation (7) does a good qualitative job of describing the mixing over a wide range of turbulence conditions. In general, the quantitative agreement is not good, but improves as the ripple factor becomes greater than 0.7. The equation is therefore very useful in predicting quickly the point where complete mixing is approached.

Model 2

Ripple factors for the three dimensional lattice of point sources are shown in figure 7. This model approximates the diffusion of a liquid which is vaporizing uniformly as it travels downstream. (As mentioned in the INTRODUCTION an exact treatment of this type of calculation is given in ref. 5.) At a turbulence intensity of 0.05 with 1/2-inch spacing, a downstream distance of 11.3 inches is now required to obtain 95 percent of perfect mixing, that is, 4 inches beyond the last downstream sources. This compares with the 5.8 inches needed for model 1. As long as sources are present downstream, the ripple factor increases rather slowly.

However, downstream of the last sources the ripple factor reaches unity in a shorter distance for the lattice model than it does for the grid of sources. This is shown by the curves in figures 4 and 7.

4834

Comparison of Mixing and Vaporization Length Calculations

The approximate mixing lengths just calculated can be compared with the results of vaporization-rate calculations reported in references 3 and 9. A comparison of the lengths required for 95-percent mixing with those required for 95-percent vaporization of the mass of typical rocket-engine sprays will give an idea of the relative importance of the two processes when they occur simultaneously. The table below summarizes calculations from references 3 and 9 for several heptane sprays and one oxygen spray evaporating into an assumed rocket-engine combustion environment.

CI-2

Mass median drop radius, in.	Standard geometric deviation, σ_g	Length for 95-percent mass vaporized, in.	
		Heptane	Oxygen
0.003	1.25	5.9	
	1.54	7.8	
	2.3	14	5.8
	3.6	25	

The larger the value of σ_g, the greater is the radius of the largest drop in the spray for a given mass median drop radius. The largest 95-percent mixing lengths found in the present calculations (at the 1/2-inch source spacing) are 5.8 inches for model 1 and 11.3 inches for model 2. This information indicates that for cases with $\sigma_g > 1.25$, gaseous mixing from a single grid of point sources is faster than vaporization of a heptane spray. Reference 3 shows that several actual injector sprays have a σ_g value of about 2.5. The conclusion is that gaseous mixing for the grid of sources model occurs in a shorter length than is needed to vaporize typical rocket-engine heptane sprays. Additional calculations in reference 9 have shown this statement to be true for fuels other than heptane. The vaporization length for the oxygen spray is the same as the maximum mixing length found for the grid of sources model. So if a fuel more volatile than oxygen is used with it, the mixing rate still does not become the limiting factor on the entire combustion rate, even at the lowest turbulence intensity used.

The mixing length calculated for a lattice of diffusion sources extending 7 inches downstream is not significantly less than the vaporization

length for a heptane spray with a σ_g value of 2.3. No quantitative significance is given to the actual values. The comparison does show that, although the mixing process is quite rapid downstream of the last diffusion sources, it is by no means fast enough to be completely neglected as a combustion-rate controlling factor.

The preceeding comparison of the rates of mixing and vaporization has been made on the basis of time-average concentration calculations. The time variation of concentration at a given point can be quite significant. (The root-mean-square value of the fluctuation can be as high as 80 percent of the mean value.) What effect these time fluctuations will have upon the mixing process is not known from the present work. (See ref. 10 for a method of treating these fluctuations.)

The several principle assumptions used in this analysis and their implications with respect to a rocket-combustion process require some further discussion:

(1) The volume occupied by the diffusing gas is assumed negligible compared with that of the main stream. In a practical case this assumption is, of course, never realized. For example, in the combustion of hydrogen and oxygen at an oxidant-fuel mass ratio of 4.0 the ratio of oxygen to hydrogen volumes is 1:4. In a constant area duct, therefore, the injection of gaseous oxygen would accelerate the total flow by approximately 25 percent.

(2) The mixing is assumed to occur between nonreacting gases. The contribution of the combustion process to the mixing is not considered. The idea of "flame-generated" turbulence was proposed several years ago, but no experimental evidence has yet been found to support the idea that combustion significantly increases the scale and intensity of turbulent flow (see refs. 11 and 12). The fact remains, however, that little is known about the effect of the combustion process on mixing.

(3) The turbulence scale and intensity are assumed to remain constant throughout the mixing process. This assumption is a direct consequence of assumption (2). Photographic studies of combustion indicate that flow downstream of the principal combustion zone is pseudolaminar (ref. 13). It seems likely that, in a real combustor, turbulence intensity diminishes rapidly beyond the main reaction zone.

SUMMARY OF RESULTS

For gaseous diffusion from groups of continuous point sources the following results are summarized:

1. Turbulent mixing is practically independent of the scale of turbulence except at very low values.

2. Mixing increases with increasing turbulence intensity and with increasing ratio of downstream distance to source spacing.

3. On the basis of these time-average concentration calculations, turbulent mixing is faster than the vaporization process for the simple grid of sources model at all the turbulence intensities used. This work has told nothing, however, about the time-dependent concentration fluctuations, which can be large enough to affect the mixing process.

4. Practically all the mixing occurs by turbulent diffusion in the models used. Molecular diffusion contributes negligibly to the mixing so that the results of the present work are independent of any particular propellant combination. This is true for source types other than the continuous point source.

Lewis Flight Propulsion Laboratory
National Advisory Committee for Aeronautics
Cleveland, Ohio, June 10, 1958

4834
Copy back

APPENDIX - ANALYTICAL EXPRESSION FOR THE RIPPLE FACTOR IN MODEL 1

Figure 1(b) shows the geometric relations for this model, as viewed along the x-axis. Only points near the center of the grid are considered. Point A is a typical point on a source streamline for the calculation of C_{max}. The most important sources contributing at this point are (1) one with $r' = 0$, (2) four with $r' = s$, and (3) four with $r' = s\sqrt{2}$. The typical point for C_{min} is point B. In this case the contributing sources are (1) four with $r = s\sqrt{2}/2$ (indicated by the squares), (2) eight sources with $r = s\sqrt{10}/2$ (indicated by the triangles), and (3) four with $r = s\sqrt{18}/2$ (indicated by the diamonds). If only these three values of r and r' are used in the general equation (6), it becomes 4834

$$\psi = \frac{4e^{-s^2/8\omega} + 8e^{-5s^2/8\omega} + 4e^{-9s^2/8\omega}}{1 + 4e^{-s^2/4\omega} + 4e^{-s^2/2\omega}} \tag{A1}$$

Next, equation (4) for ω can be simplified by dropping the molecular diffusion term, expanding the exponential, and dropping all terms above second order. The result is

$$\omega = \frac{x^2T^2}{2} \tag{A2}$$

Substitution of equation (A2) into equation (A1) gives

$$\psi = \frac{4e^{-1/4\alpha^2} + 8\left(e^{-1/4\alpha^2}\right)^5 + 4\left(e^{-1/4\alpha^2}\right)^9}{1 + 4\left(e^{-1/4\alpha^2}\right)^2 + 4\left(e^{-1/4\alpha^2}\right)^4} \tag{7}$$

REFERENCES

1. Penner, S. S., and Datner, P. P.: Combustion Problems in Liquid-Fuel Rocket Engines. Fifth Symposium (International) on Combustion, Reinhold Pub. Corp., 1955, pp. 11-29.

2. Priem, Richard J.: Propellant Vaporization as a Criterion for Rocket-Engine Design; Calculations of Chamber Length to Vaporize a Single n-Heptane Drop. NACA TN 3985, 1957.

3. Priem, Richard J.: Propellant Vaporization as a Criterion for Rocket-Engine Design; Calculations Using Various Log-Probability Distributions of Heptane Drops. NACA TN 4098, 1957.

4. Heidmann, Marcus F., and Priem, Richard J.: Propellant Vaporization as a Criterion for Rocket-Engine Design; Relation Between Percentage of Propellant Vaporized and Engine Performance. NACA TN 4219, 1958.

5. Scull, Wilfred E., and Mickelsen, William R.: Flow and Mixing Processes in Combustion Chambers. Ch. II of Basic Considerations in the Combustion of Hydrocarbon Fuels with Air. NACA Rep. 1300, 1957.

6. Mickelsen, William R.: An Experimental Comparison of the Lagrangian and Eulerian Correlation Coefficients in Homogeneous Isotropic Turbulence. NACA TN 3570, 1955.

7. Longwell, John P. and Weiss, Malcolm A.: Mixing and Distribution of Liquids in High-Velocity Air Streams. Ind. and Eng. Chem., vol. 45, no. 3, Mar. 1953, pp. 667-677.

8. Hirschfelder, Joseph O., Curtiss, Charles F., and Bird, R. Byron: Molecular Theory of Gases and Liquids. John Wiley & Sons, 1954, p. 539.

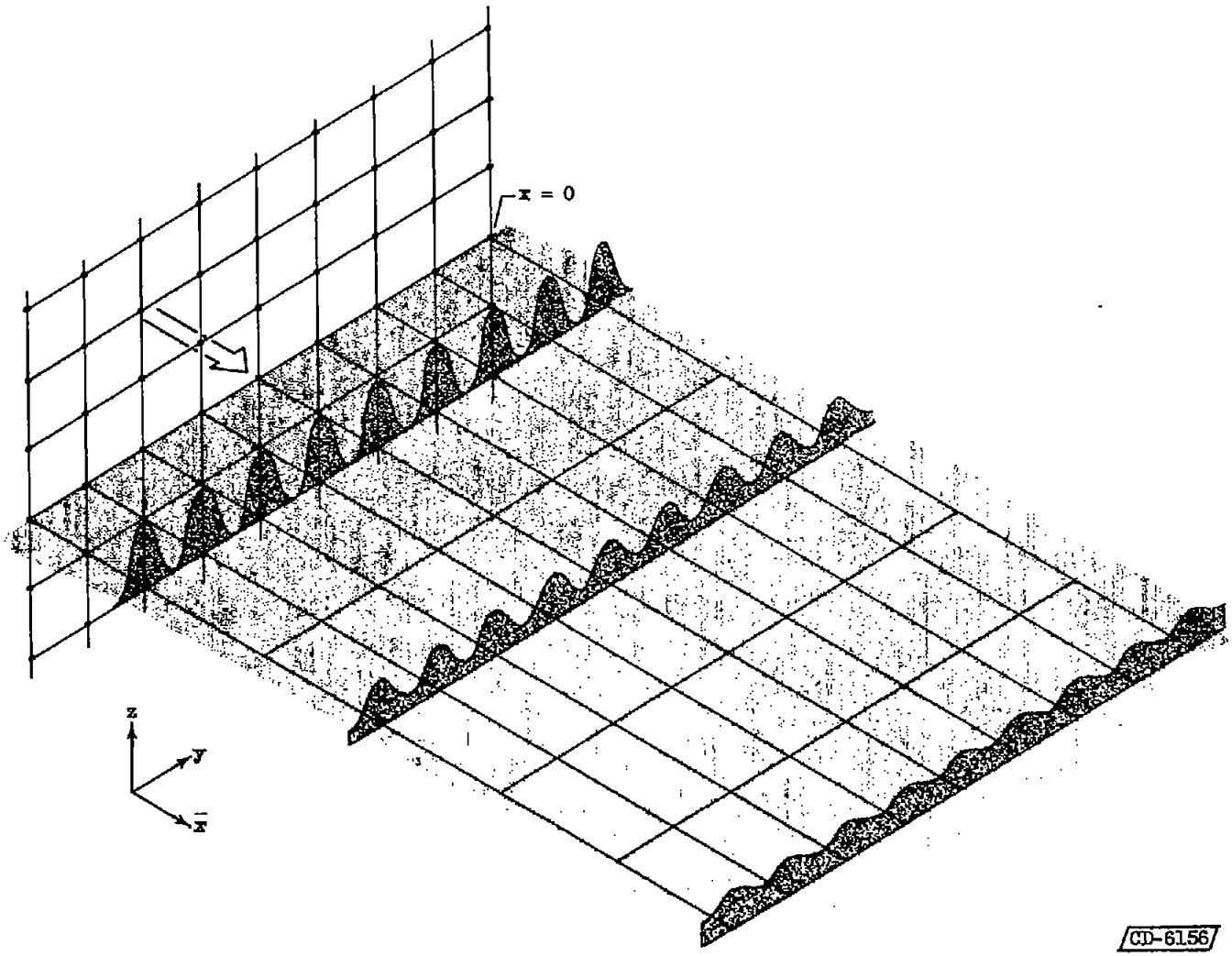
9. Priem, Richard J.: Propellant Vaporization as a Criterion for Rocket-Engine Design; Calculations of Chamber Length to Vaporize Various Propellants. NACA TN 3883, 1958.

10. Uberoi, M. S., and Corrsin, S.: Diffusion of Heat from a Line Source in Isotropic Turbulence. NACA Rep. 1142, 1953. (Supersedes NACA TN 2710.)

11. Richmond, J. Kenneth, et al.: Turbulent Burning Velocities of Natural Gas-Air Flames with Pipe Flow Turbulence. Sixth Symposium (International) on Combustion, Reinhold Pub. Corp., 1957, pp. 303-311.

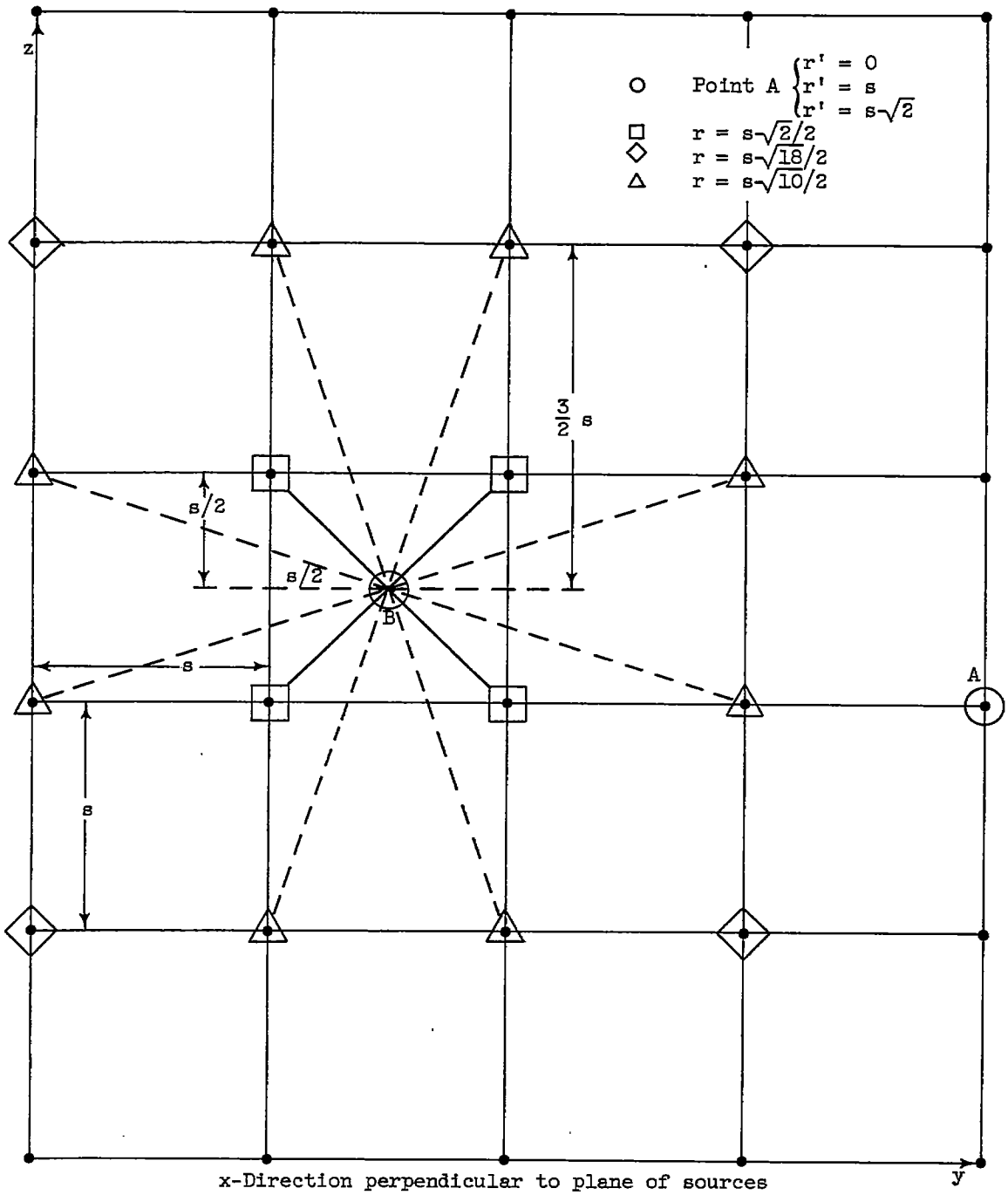
12. Westenberg, Arthur A.: Flame Turbulence Measurements by the Method of Helium Diffusion. Jet Prop., vol. 26, no. 6, June 1956, p. 481.

13. Bellman, Donald R., Humphrey, Jack C., and Male, Theodore: Photographic Investigation of Combustion in a Two-Dimensional Transparent Rocket Engine. NACA Rep. 1134, 1953. (Supersedes NACA RM E8F01.)



(a) Perspective view.

Figure 1. - Diffusion model for a grid of evenly spaced point sources, model 1.



(b) Geometric relations.

Figure 1. - Diffusion model for a grid of evenly spaced point sources, model 1.

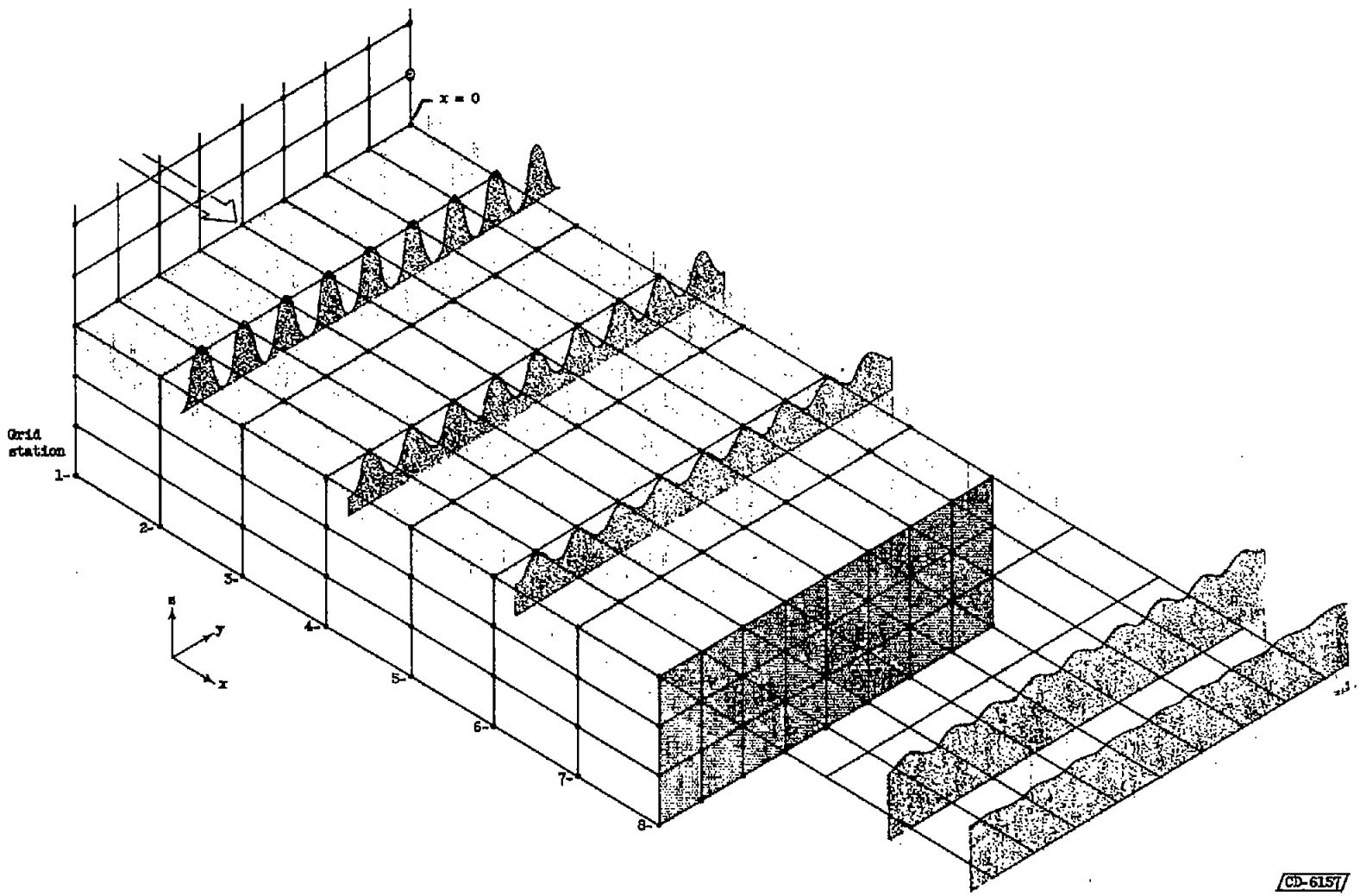
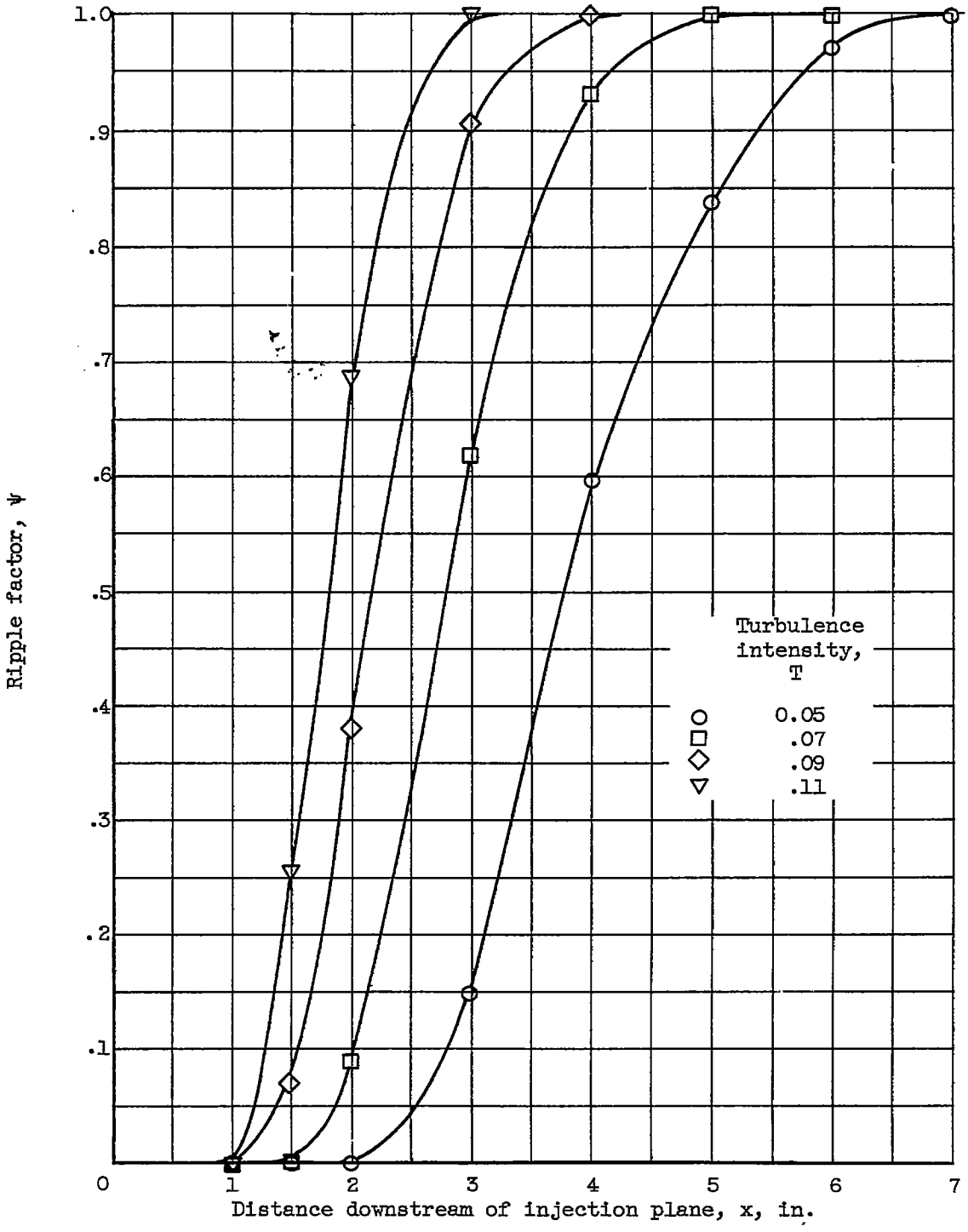
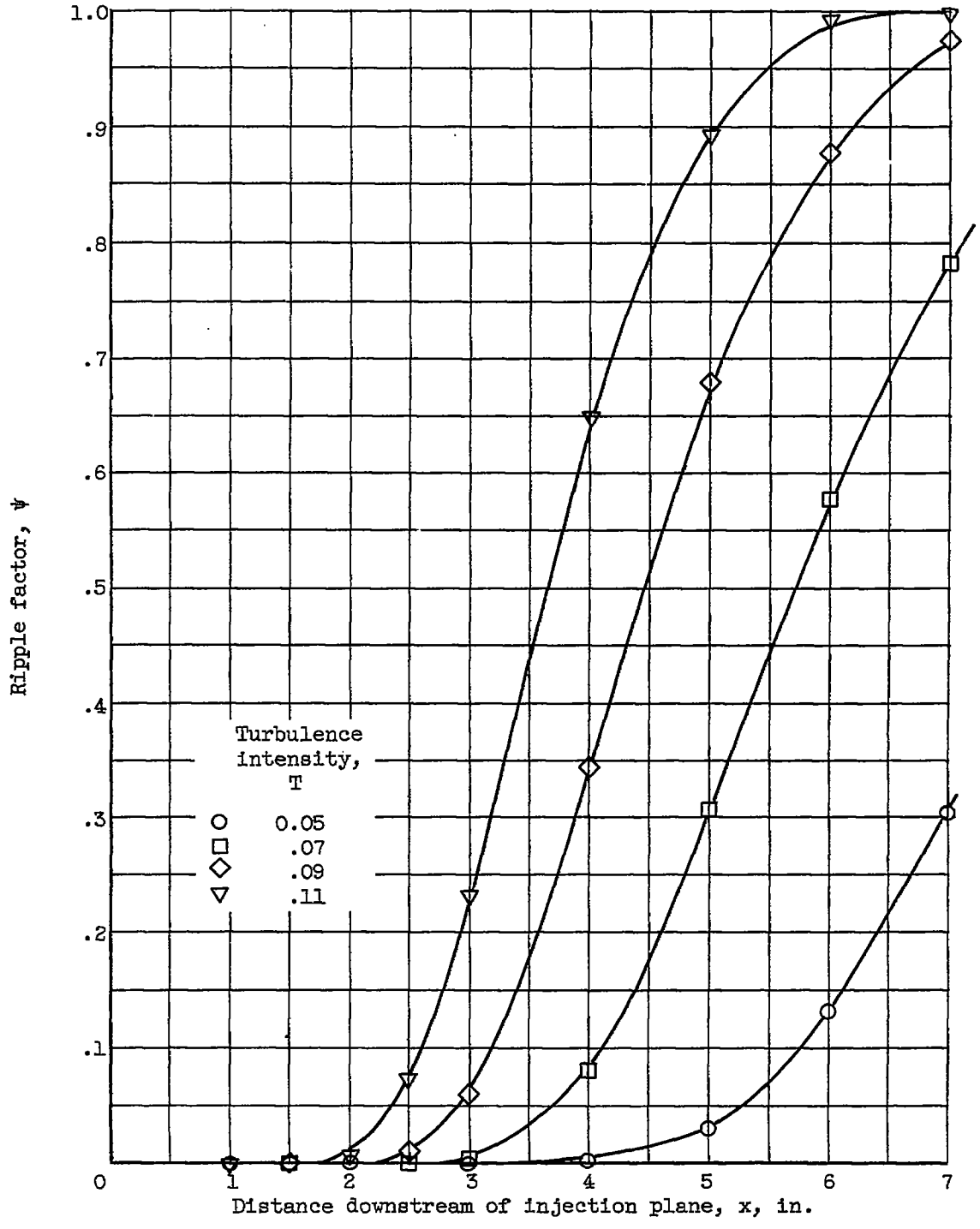


Figure 2. - Diffusion model for a lattice of point sources, model 2.



(a) Source spacing, 1/2 inch.

Figure 3. - Ripple factor against downstream distance for the grid of sources, model 1. Turbulence scale, 0.10 foot.



(b) Source spacing, 1 inch.

Figure 3. - Concluded. Ripple factor against downstream distance for the grid of sources, model 1. Turbulence scale, 0.10 foot.

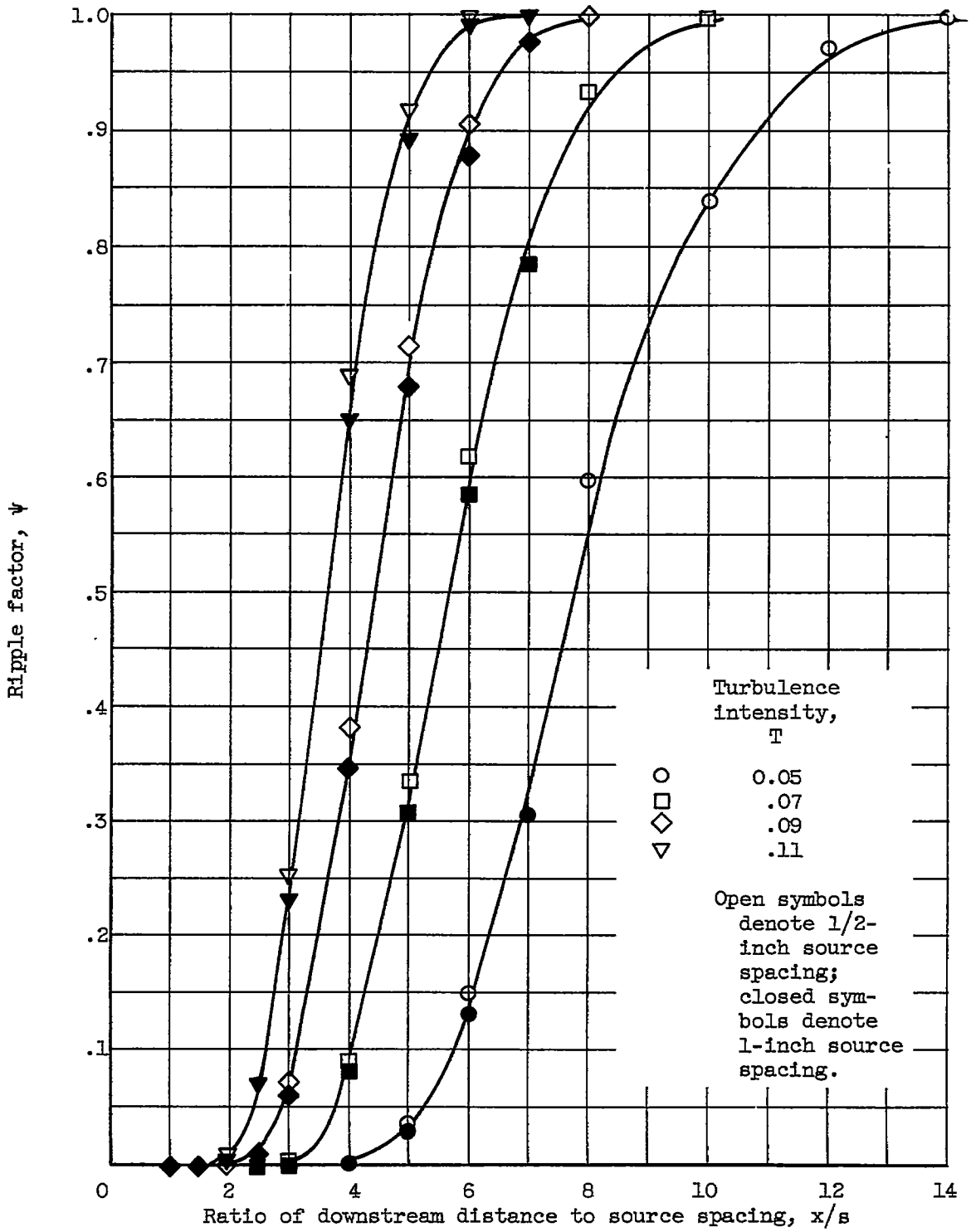


Figure 4. - Ripple factor against distance to spacing ratio for model 1.

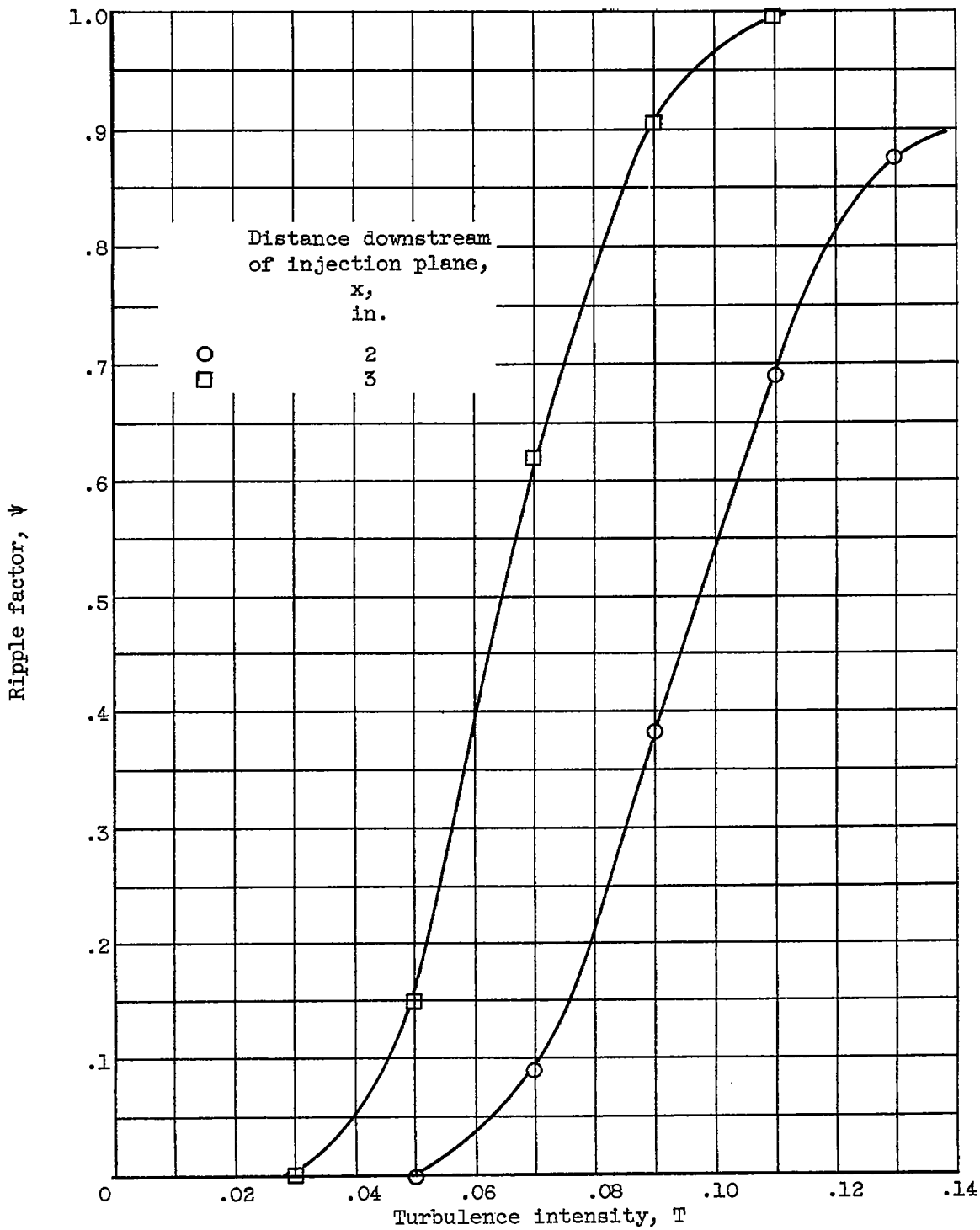


Figure 5. - Ripple factor against turbulence intensity for the grid of sources, model 1.

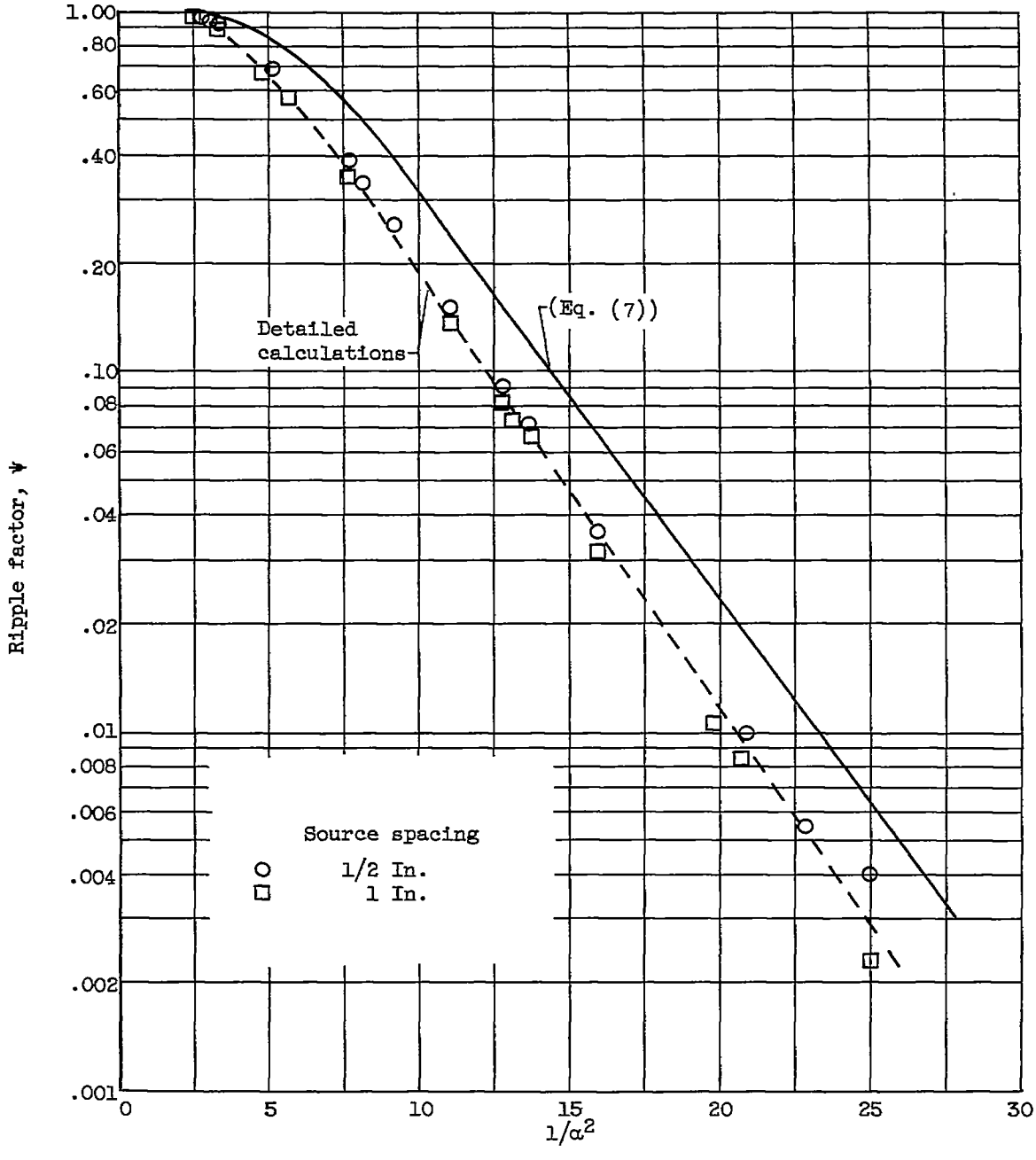


Figure 6. - Approximate ripple factor equation for model 1.

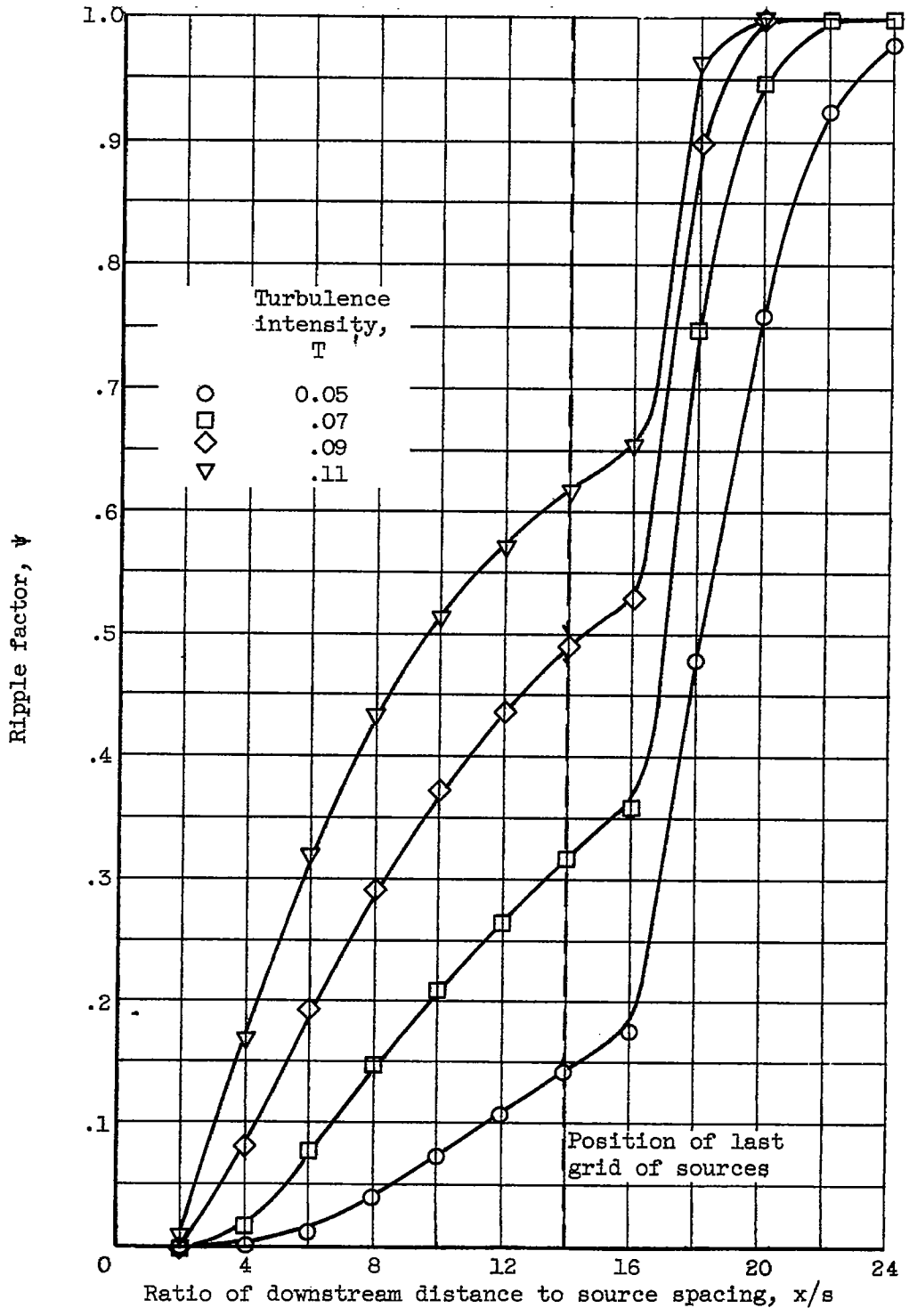


Figure 7. - Ripple factor against distance to spacing ratio for model 2; source spacing (in y-z plane), 1/2 inch.