NASA TECHNICAL MEMORANDUM

NASA TM X-53112

August 20, 1964

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MONTE CARLO SOLUTIONS OF KNUDSEN AND NEAR-KNUDSEN FLOW THROUGH INFINITELY WIDE, PARALLEL AND SKEWED, FLAT PLATES

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ABSTRACT

This study presents the results of an investigation of Knudsen flow and near-Knudsen flow through infinitely wide, parallel and skewed, flat plates. Monte Carlo computer techniques were used. Two simple models for considering molecule-molecule interactions, as well as molecule-surface interactions, were used to examine the near-Knudsen flow regime. Transmission probabilities for various length-to-entrance ratios and for various angles of skewness are presented. The influence of mean free path and length-to-entrance ratios on Knudsen flow determination is discussed.

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AERO-ASTRODYNAMICS LABORATORY
RESEARCH AND DEVELOPMENT OPERATIONS

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DEFINITION OF SYMBOLS

Symbol	Definition
A	distance between plates at opening
A_o	A/2, y value of surface at x = 0
A_L	y value of surface at x = L
L	length of plates
N	local normal
X_+, Y_+	x and y coordinates of the point of collision with the upper plate
X_-, Y_-	x and y coordinates of the point of collision with the lower plate
x_1, y_1	coordinates of random point on the entrance line
θ	angle between the local normal and the molecule path
φ	angle between the molecule path and the positive x-axis
δ_+, δ_-	angle of divergence or convergence of the surfaces with respect of positive x-axis
ϵ	angle of divergence or convergence of the surface with respect to parallel plate configuration

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SUMMARY

This study presents the results of an investigation of Knudsen flow and near Knudsen flow through infinitely wide, parallel and skewed, flat plates. Monte Carlo computer techniques were used. Two simple models for considering molecule-molecule interactions, as well as molecule-surface interactions, were used to examine the near-Knudsen flow regime. Transmission probabilities for various length-to-entrance ratios and for various angles of skewness are presented. The influence of mean free path and length-to-entrance ratios on Knudsen flow determination is discussed.

I. INTRODUCTION

The study of rarefied gas dynamics has become of increasing interest to many areas of scientific and engineering problems other than that of low density aerodynamics. This is evident from the studies for space simulation chamber design, measurements of vapor pressures of materials, design of ion engine thrust chambers, etc. The region which is of most interest and which has been investigated most thoroughly is the regime of free-molecule flow (or Knudsen flow). Free-molecule flow is characterized by densities so low that intermolecular collisions can be ignored, and only collisions with surfaces need be considered. Solutions to general free molecule flow problems can be found in most texts on kinetic theory; however, many detailed studies have been conducted by a large number of investigators. Perhaps the most interesting parameter of Knudsen flow is the transmission probability; that is, the probability that a molecule will pass through the configuration under study. Because P. Clausing [1] conducted extensive investigations of this parameter, transmission probabilities are generally called Clausing factors.

Most investigators today continue to use Clausing's approach to problems in free molecule flow. In 1960, D. H. Davis [2] demonstrated the use of Monte Carlo computer methods to determine Clausing factors for simple and complex geometries. Since that time, other investigators have used this approach for such studies [3, 4, 5]. Several years ago the writer felt that the Monte Carlo studies might offer a significant advantage in the study of free molecule and transition flow regimes. By

following the collisions of molecules with the walls and with other molecules, perhaps better insight of the importance of parameters such as reflection coefficients, energy accommodation coefficients, momentum accommodation coefficients, sticking coefficients, capture coefficients, etc., could be obtained. Accordingly, several studies and computer programs were initiated. Some of these results have been published [4, 5]. Present studies include the determination of transmission probabilities through infinitely wide, parallel and skewed, flat plates; rectangular ducts; and circular tubes including effects of other parameters such as speed ratios (the ratio of mass velocity to the most probable molecular velocity), angle of attack, mean free path, etc. These studies are being published in a series of reports of which this is the first. This paper presents the transmission probabilities through infinitely wide, parallel and skewed, flat plates as a function of the length of the plates and the angle of skewness. No data for speed ratios or angle of attack are given at this time. Results from an early series of mean free path studies are presented.

The author is deeply indebted to Mr. David W. Tarbell for his interest and participation in the development of the techniques, ideas and programs used for this study. Through this acknowledgement, the writer wishes to recognize the effort which he has expended in these studies. Also the author is indebted to Mr. Raymond Smith who patiently incorporated the many changes into his computer programs.

II. ASSUMPTIONS AND PROCEDURES

Typical of any study of free molecule flow are the assumptions: (1) that only molecule-surface collisions need be considered and (2) that, after colliding with a surface, the molecules are reflected diffusely. The model for this study can be envisioned as infinitely wide, flat surfaces connected to two semi-infinite large vessels, one at some low density ρ and the other at a perfect vacuum. Thus, the flow will be from the vessel with density ρ to the other vessel and no molecules will reenter the system. While this situation is not physically possible, it suffices for the determination of transmission probabilities. This condition specifies that molecules enter the volume of interest with a cosine distribution with respect to the plane of the opening. Also, since the plates are infinitely wide, one need not consider the third dimension, and two-dimensional solutions may be used. (The assumption is also verified by the rectangular duct studies to be reported later. Using a three-dimensional study, one can obtain the same results as the two-dimensional study when one considers a wide rectangular duct.)

The actual program is a very simple procedure. A random position on the entrance plane (a line in two-dimensions) is generated, and the direction cosines are randomly generated (but constrained with the diffuse reflection concept). The molecule is then tested to see if it will pass through the system or collide with the surfaces. If a collision occurs, the coordinates of the collision are determined, new direction cosines are generated, and the molecule is again tested to see if it passes through the system (at either exit) or if it collides again. The molecule is followed until it exits the system or until a specified number of collisions are made. Although this specific number of collisions can be any value, it usually ranged from 20 to 100, depending on the length-to-opening ratio of the plates. For large length-to-opening ratios, a significant number of molecules make over 100 collisions without exiting the system. Analysis of computer results indicates that sufficient accuracy is obtained by following the history of 10,000 molecules. Results are tabulated with respect to the exit plane and the number of collisions.

To consider intermolecular collisions, the same procedure is used except that, for a given mean free path, random free paths are generated consistent with the distribution of free paths for the specified mean free path. The molecule path length is then calculated and compared with the free path. If the molecule path becomes longer than the free path before the molecule exits the system, a collision is assumed, and the coordinates of the position of the molecule when its path equals the free path are calculated. The molecule is then randomly scattered from that point, a new free path is generated, and the procedure continues. For this initial study, molecular collisions with the wall are not considered to change the free path length.

III. PROGRAM DESCRIPTION

The details of the computer programs for the flat plates can be most easily understood by referring to Figure 1. Molecules are assumed to enter from the right uniformly along the x = 0 line. The initial coordinate y is calculated from the expression

$$Y = A_o(1 - 2R_1)$$

where R is a random number between 0 and 1.0. (For convenience, all results are expressed in terms of the ratio of length to opening.)

The angle φ is given by

$$\varphi = 180° + \theta,$$

where θ is given by

$$\sin \theta = (1 - 2R_2).$$

The equation for the $Y_2 = \tan \varphi \, (X_2) + Y_1$ is then generated and tested to see if it intersects with the surfaces or with the exit line $x = L$. If the molecule exits, the event is recorded and a new molecule is started. If a collision with the surface occurs, the coordinates of the intersection are calculated from

$$X_{\pm} = \frac{\pm A_o - L \tan \varphi - Y_2}{\tan \varphi - \tan \delta \, (\pm)}$$

$$Y_{\pm} = (\tan \delta_{\pm}) \, (X_{\pm}) \pm A_o,$$

where the + and - signs refer to the upper and lower plates, respectively. New direction cosines are generated and the molecule is tested again, this time to see if it exits either opening or collides with the surfaces. If it exits, it is categorized by the plane of exit and the number of collisions. If it does not exit, the new intersection coordinates are calculated and the procedure is repeated. The molecules can be followed for any number of collisions, but normally are limited to 20, 50, or 100 collisions. A flow diagram for the program showing the most significant logic blocks is presented in Figure 2.

IV. RESULTS

A. Free Molecular Flow

The transmission probability factor, K_{mc}, for infinitely wide, parallel and skewed, flat plates is presented graphically in Figures 3 through 9. Figure 3 shows these factors as a function of the length-to-entrance ratio for parallel plates. Also shown on this figure are

Clausing's data. Figures 4 through 6 present the K_{mc} values for skewed flat plates diverging from the direction of flow, while Figures 7 through 9 show the K_{mc} values for the converging plates. It must be remembered that in both cases molecules are entering the system uniformly. Figure 10 presents the K_{mc} values as a function of the angles of divergence. It is easily seen from this figure that a small angle of divergence rapidly increases the transmission probability of the system. Also one should expect, it is easily seen that for all L/A values and large angles of divergence, the K_{mc} values approach 1.0 rapidly.

Tables I, II, and III show the fraction of molecules exiting the system. These tables are the L/A values of 1, 2, and 5 and show the fraction of molecules which leave the array at the exit plane X_L and which leave at the entrance plane X_O. It is obvious for the column X_O (corresponding to the entrance plane) that no molecules can exit without at least one collision with the flat plates. The designation "out" is used to show the fraction of molecules making more collisions than those listed in the tables.

B. Transition Flow

Using the simple approach explained earlier, the mean free path was varied to provide Knudsen numbers (based on the entrance value A for a parallel plate system with L/A = 1) from 0.1 to 1000. The K_{mc} values from this approach are presented in Figure 11 and are plotted against the Knudsen number. Also shown is the Clausing factor for L/A = 1. Perhaps the most noticeable feature of this figure is the fact that the data approach the Clausing factor only when K_n is greater than 30. Another interesting feature from the computer data is that, for a Knudsen value of 10, approximately 13 percent of the molecules had one intermolecular collision, 1 percent had two intermolecular collisions, and .1 percent had three collisions. For a Knudsen number of one only about 29 percent of the molecules passed through the array without at least one collision with another molecule. Figure 14 shows normalized transmission probabilities for several L/A values.

V. DISCUSSION OF ACCURACY

The easiest way to estimate the accuracy of the Monte Carlo solutions is to compare the results with Clausing's results. DeMarcus [6] has shown that Clausing's results are at least 0.1 percent accurate. The Monte Carlo solutions do not approach that degree of accuracy. Figure 12 presents Monte Carlo solutions of transmission probabilities for parallel plates with an L/A ratio of 2. Ten different sets of random numbers were used to generate these values. The Clausing solution is .4517 and is given by the solid line. Dotted lines above and below the

Clausing solution indicate the ±1 percent and ±2 percent values around Clausing solution. The K_{mc} values for the ten runs are also plotted. It is readily seen that the solutions are usually within ±1 percent.

Another method which can be used to check the accuracy of the computer program is based on the grouping of the results by collision number and the analogy between radiant heat transfer and free molecular flow. Since the molecules are assumed to enter uniformly over the entrance plane and have a cosine distribution with respect to that plane, the fraction of molecules which passed through the system and exit without making a collision, should be equal to the form factor for radiant heat transfer between the entrance and exit planes. From the ten solutions used in Figure 12, the fraction of molecules which make no collisions is plotted in Figure 13. The form factor for this configuration is .2361. Also shown are the ±1 percent and ±2 percent values around the form factor value. Again, it can be seen tha the computer values are near the ±1 percent value range.

VI. CONCLUSIONS AND DISCUSSION

Monte Carlo solutions of transmission probabilities for free molecular flow through infinitely wide, parallel and skewed, flat surfaces have been presented. In addition to the gross results which the transmission probabilities represent, further insight into the physical properties of the flow was gained by tracking the molecules and recording their collisions with the walls and with other molecules. It is believed that the greatest advantage of Monte Carlo solutions lies in the fact that the amount of information which one can gain from this type of approach is limited only by the ingenuity of the investigator and the available computer time.

While it has been demonstrated that most Monte Carlo solutions seem to be 1 percent to 2 percent accurate when compared to other solutions, the writer does not wish to imply that one could obtain a Monte Carlo solution and expect the results each time to be that accurate. No single result can be judged independent of the family of solutions and have this level of confidence. Quite often data with much larger errors are generated, but, when the family of data is analyzed, those errors are conspicious and can be avoided.

The simple model for the transition or near-Knudsen flow is most likely in error. It is felt that, when the molecule strikes a wall, it will be emitted in a manner independent of its previous path (at least, at low molecular velocities with respect to the wall). Therefore, a new free path length should be assigned to it. This has been tested in the present study, and, for the short ducts considered in Figure 14, there are no noticeable changes in the results. It is expected that for longer

ducts (i.e., L/A values of about 10) noticeable differences will appear. These results will be published later. Also, the molecule-molecule collision dynamics are certainly oversimplified at this time. Introduction of persistence of velocities, density gradients, etc., is being incorporated into the study.

TABLE I

FRACTION OF MOLECULES EXITING SYSTEM AS A FUNCTION OF THE NUMBERS OF COLLISION

L/A = 1.0

Values for Angle ϵ

Collision Number	0		+5		+10	
	X_L	X_o	X_L	X_o	X_L	X_o
0	.4164	0	.4748	0	.5319	0
1	.1552	.1883	.1640	.1556	.1702	.1232
2	.0675	.0714	.0699	.0584	.0685	.0434
3	.0297	.0300	.0275	.0205	.0237	.0156
4	.0132	.0118	.0098	.0082	.0083	.0063
5	.0048	.0051	.0037	.0029	.0042	.0013
6	.0017	.0019	.0017	.0010	.0013	.0011
7	.0011	.0009	.0009	.0003	.0004	.0001
8	.0006	.0003	.0003	.0000	.0002	.0002
9		.0001	.0002	.0001		.0001
10			.0000			
11			.0001			
12						
13						
14						
15				.0001		
TOTALS	.6902	.3098	.7529	.2471	.8087	.1913

TABLE II

FRACTION OF MOLECULES EXITING SYSTEM AS A FUNCTION OF THE NUMBER OF COLLISIONS

L/A = 2.0

Collision Number	Values for Angle ϵ					
	0		+5		+10	
	X_L	X_o	X_L	X_o	X_L	X_o
0	.2407	0	.3076	0	.3848	0
1	.0922	.2069	.1225	.1713	.1536	.1383
2	.0687	.1029	.0865	.0791	.0946	.0559
3	.0516	.0580	.0547	.0435	.0509	.0287
4	.0334	.0311	.0336	.0210	.9394	.0141
5	.9215	.0236	.0202	.0121	.0160	.0070
6	.0132	.0140	.0107	.0080	.0081	.0043
7	.0082	.0081	.0076	.0057	.0038	.0021
8	.0050	.0049	.0030	.0024	.0025	.0013
9	.0031	.0031	.0023	.0025	.0016	.0004
10	.0013	.0014	.0014	.0015	.0007	
11	.0018	.0009	.0009	.0009	.0007	.0001
12	.0017	.0003	.0003	.0002		
13	.0001	.0005			.0001	
14	.0004	.0002		.0001		
15	.0003	.0005	.0002			
16	.0001		.0001			
17		.0002		.0001		
18						
19						
20						
Out	.0001					
TOTALS	.5433	.4566	.6516	.3484	.7478	.2522

TABLE III

FRACTION OF MOLECULES EXITING SYSTEM AS A FUNCTION OF THE NUMBER OF COLLISIONS

L/A = 5.0

Values for Angle ϵ

Collision Number	0		+5		+10	
	X_L	X_o	X_L	X_o	X_L	X_o
0	.1015	0	.1878	0	.2711	0
1	.0199	.2156	.0525	.1672	.903	.1353
2	.0240	.1106	.0524	.0838	.0790	.0621
3	.0198	.0629	.0532	.0504	.0651	.0352
4	.0247	.0504	.0433	.0359	.0507	.0252
5	.0211	.0366	.0359	.0218	.0363	.0168
6	.0197	.0275	.0313	.0169	.0269	.0016
7	.0148	.0252	.0225	.0127	.0216	.0071
8	.0166	.0192	.0211	.0997	.0151	.0067
9	.0139	.0135	.0143	.0077	.0107	.0025
10	.0132	.0135	.0135	.0071	.0078	.0018
11	.0072	.0107	.0066	.0045	.0030	.0021
12	.0094	.0105	.0080	.0032	.0034	.0010
13	.0079	.0080	.0042	.0036	.0019	.0008
14	.0053	.0059	.0040	.0017	.0017	.0011
15	.0065	.0049	.0039	.0012	.0017	.0003
16	.0042	.0047	.0028	.0017	.0009	.0002
17	.0030	.0039	.0016	.0011	.0004	.0002
18	.0043	.0031	.0011	.0014	.0009	.0003
19	.0030	.0022	.0004	.0014	.0001	
20	.0017	.0020				
Out			.0070		.0011	
TOTALS	.3545	.6449	.5604	.4326	.6886	.3103

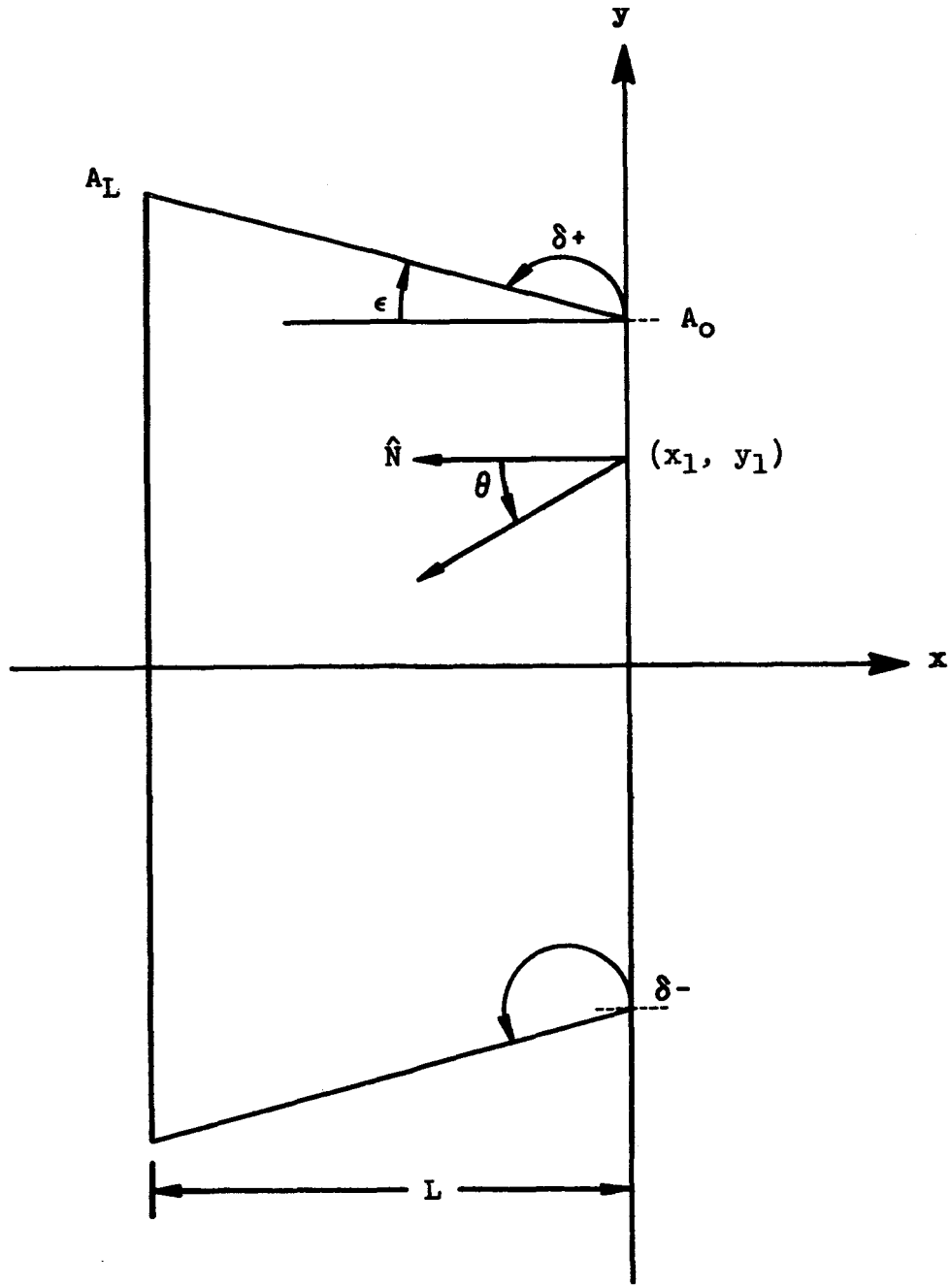

FIG. 1. BASIC CONFIGURATION FOR COMPUTER PROGRAMS

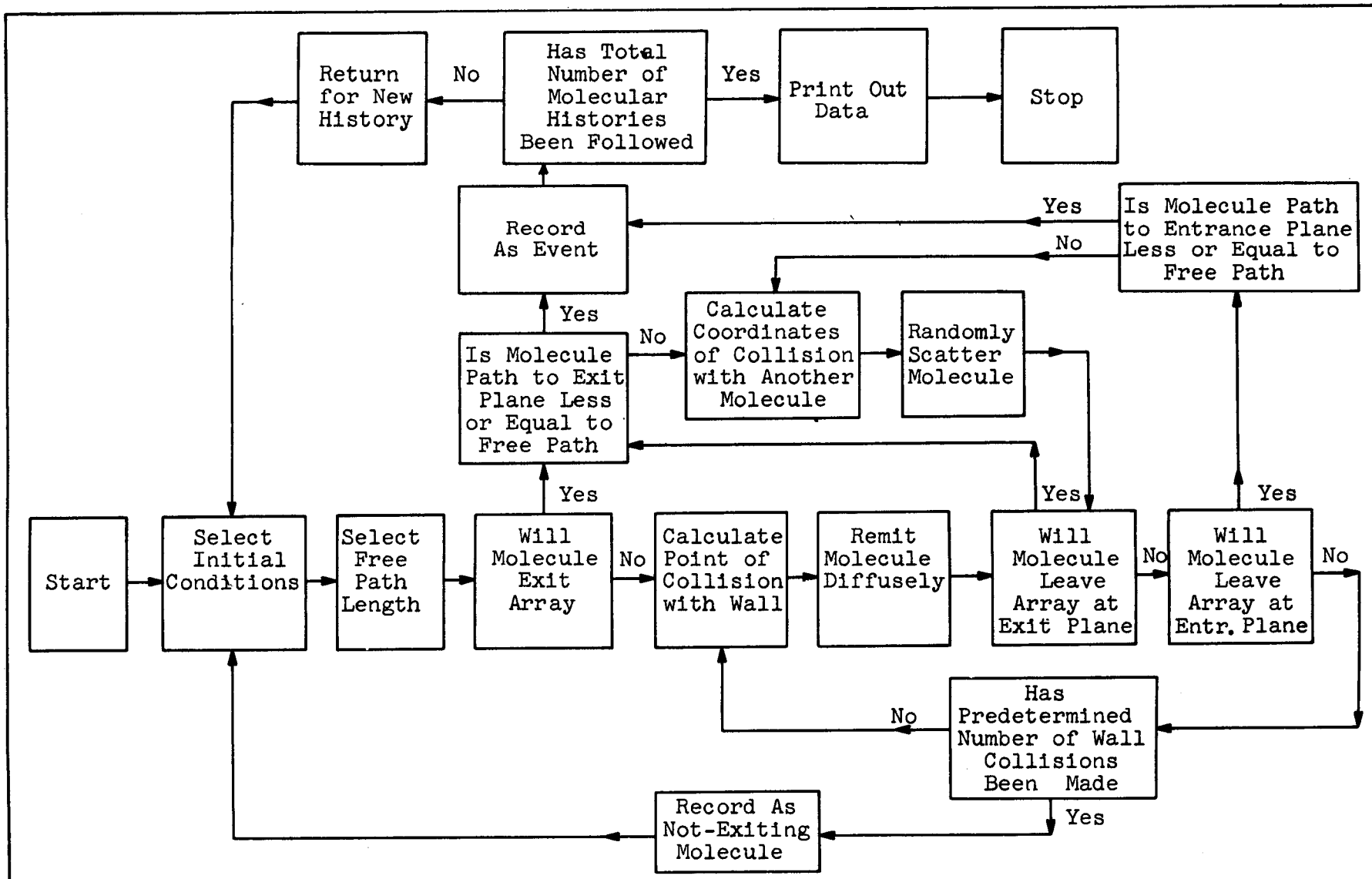

FIG. 2. FLOW DIAGRAM FOR MONTE CARLO SOLUTIONS OF TRANSMITTION PROBABILITIES INCLUDING MEAN FREE PATH INVESTIGATIONS

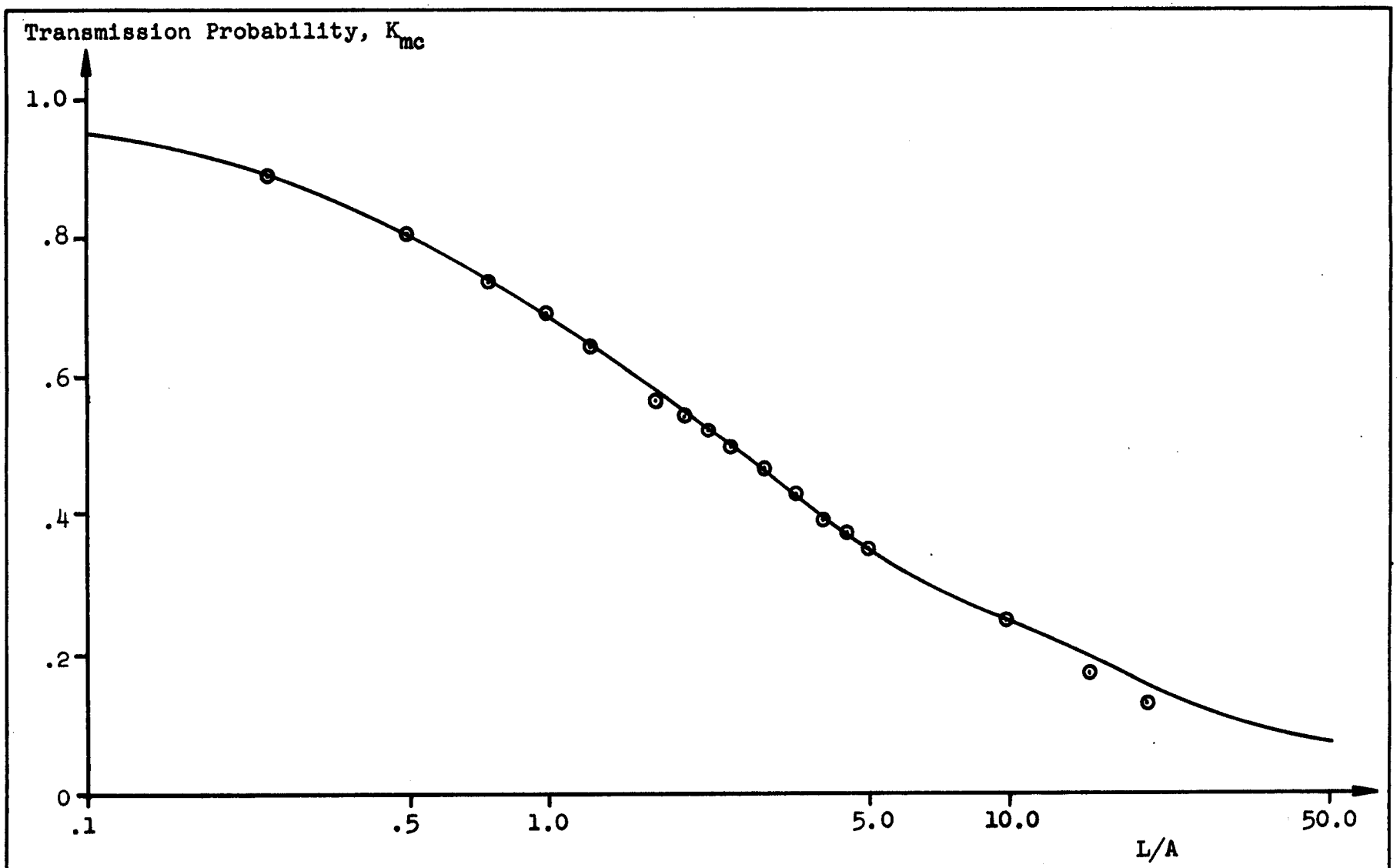

FIG. 3. TRANSMISSION PROBABILITIES, K_{mc}, FOR VARIOUS L/A VALUES FOR INFINITELY WIDE, PARALLEL FLAT PLATES. SOLID LINE REPRESENTS CLAUSING'S DATA.

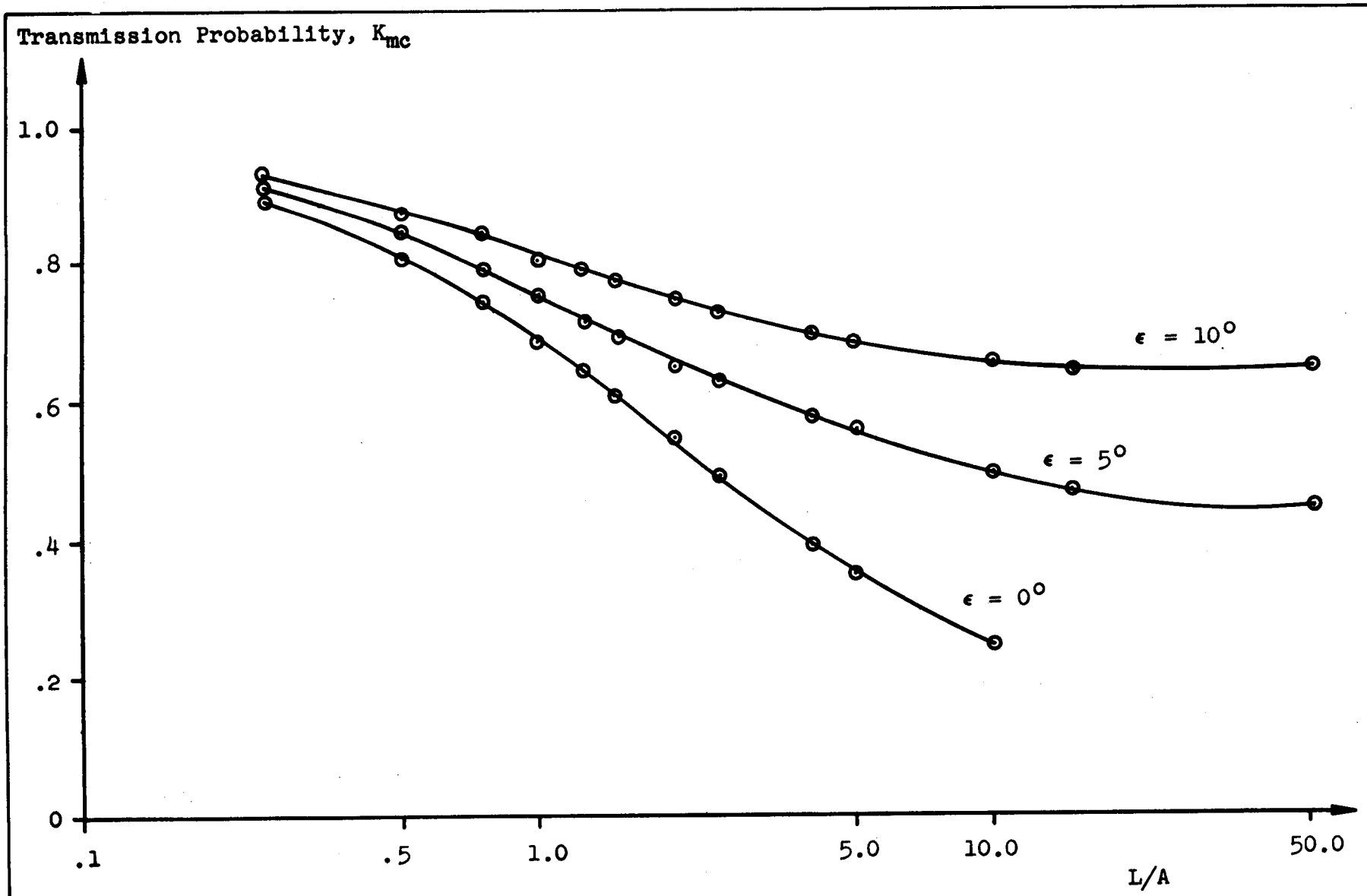

FIG. 4. TRANSMISSION PROBABILITIES, K_{mc},
FOR INFINITELY WIDE, DIVERGING FLAT PLATES FOR VARIOUS L/A VALUES.

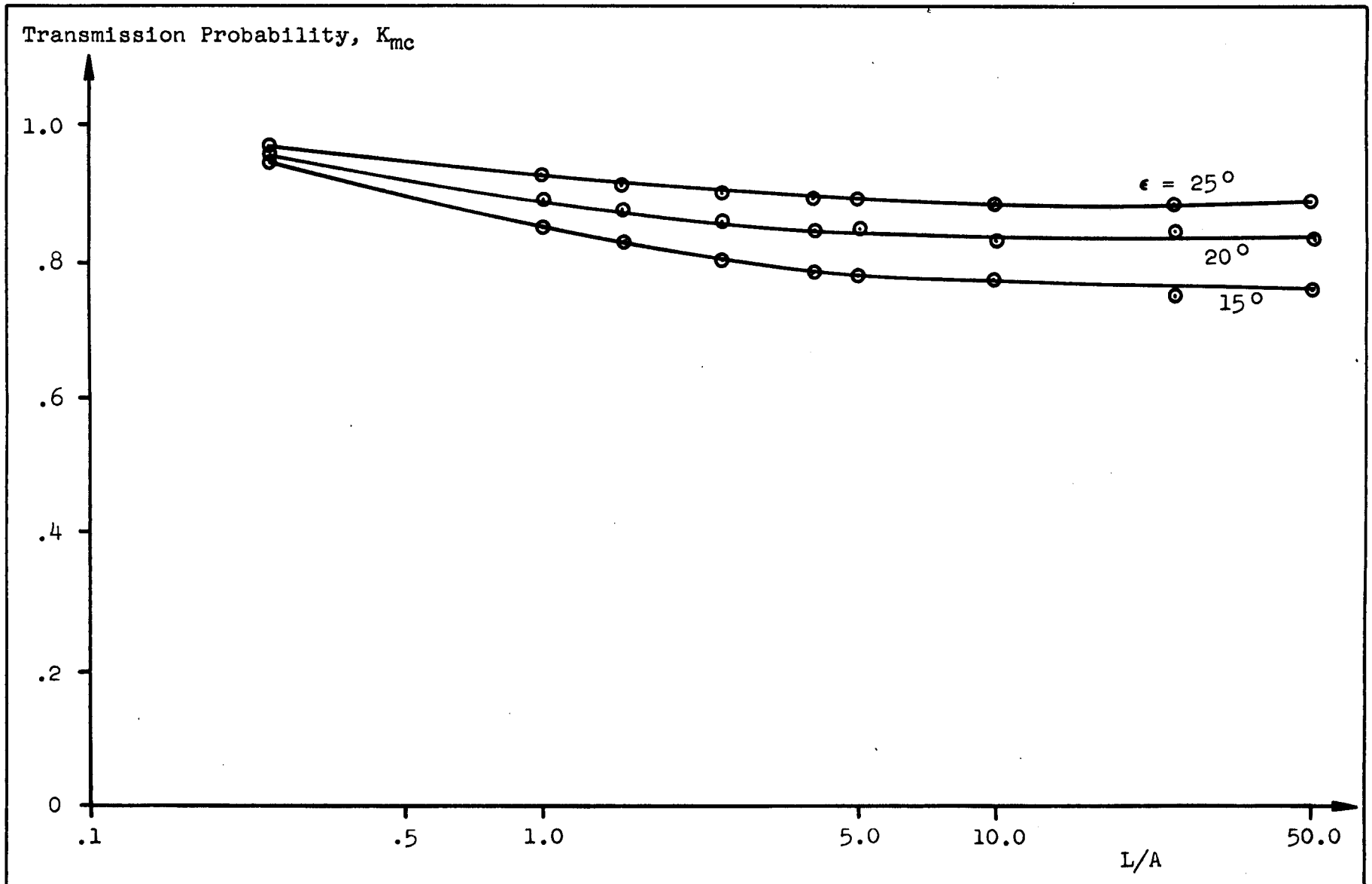

FIG. 5. TRANSMISSION PROBABILITIES, K_{mc},
FOR INFINITELY WIDE, DIVERGING FLAT PLATES FOR VARIOUS L/A VALUES.

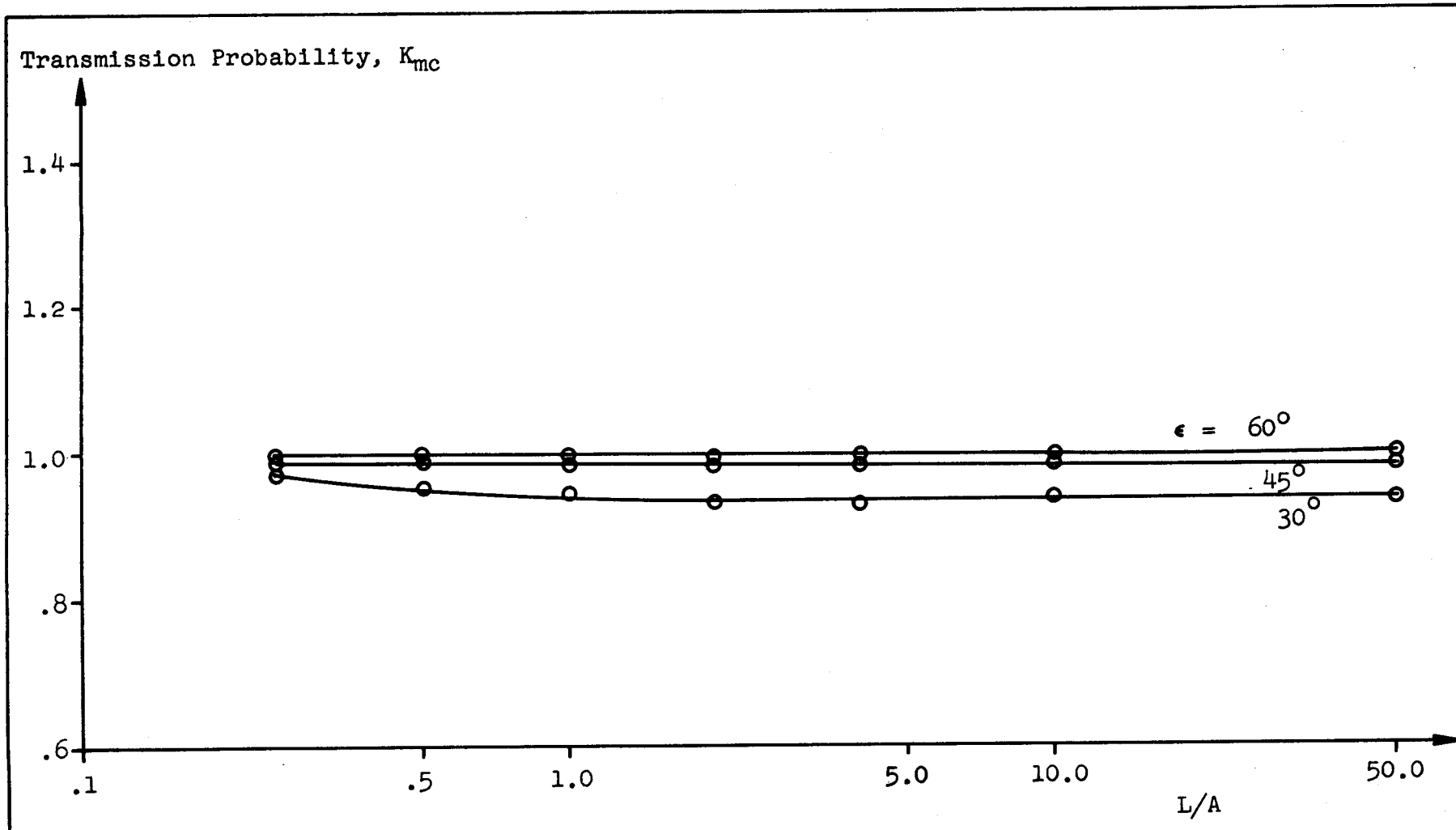

FIG. 6. TRANSMISSION PROBABILITIES, K_{mc},

FOR INFINITELY WIDE, DIVERGING FLAT PLATES FOR VARIOUS L/A VALUES.

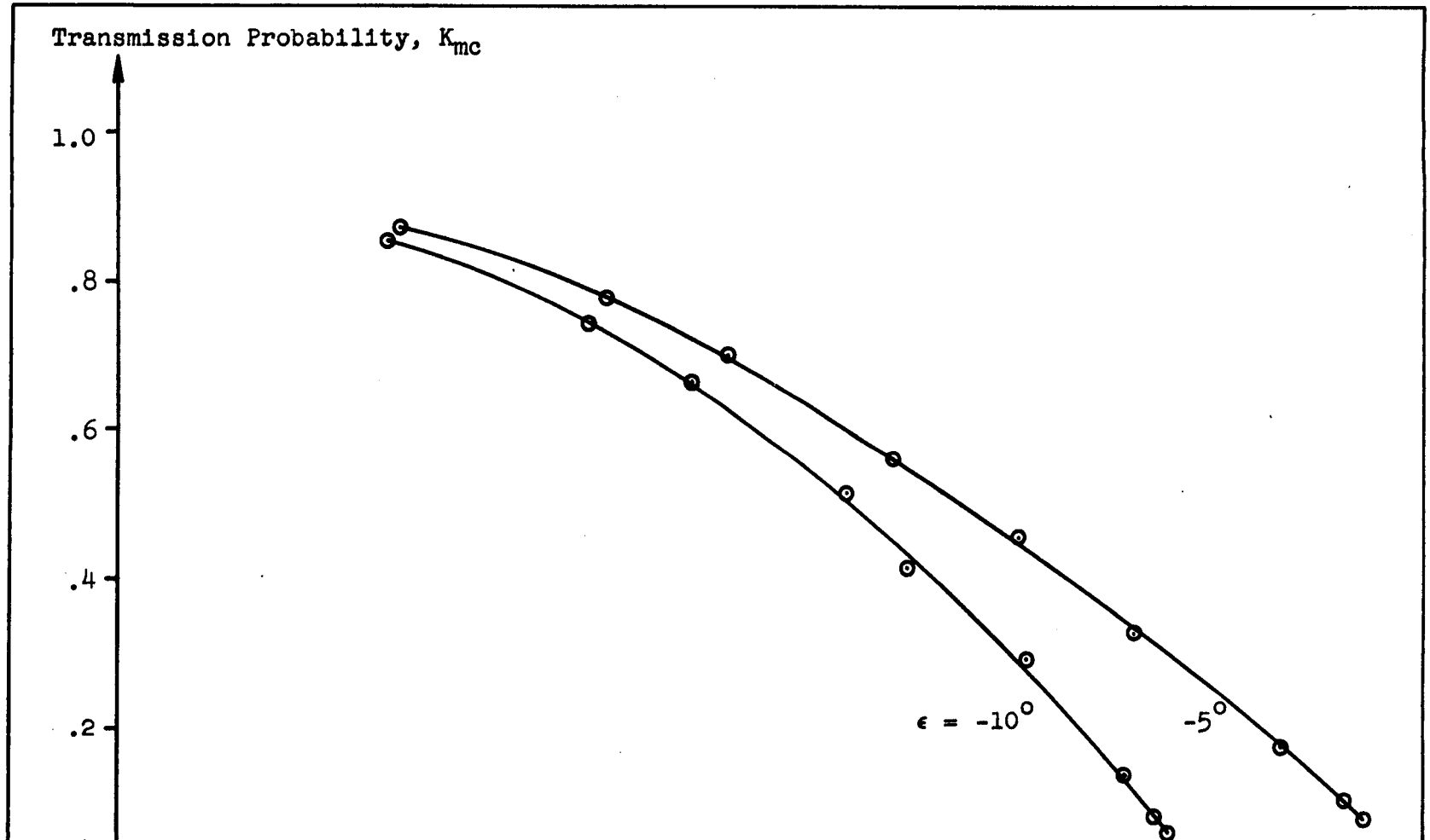

FIG. 7. TRANSMISSION PROBABILITIES, K_{mc},
FOR INFINITELY WIDE, CONVERGING FLAT PLATES FOR VARIOUS L/A VALUES.

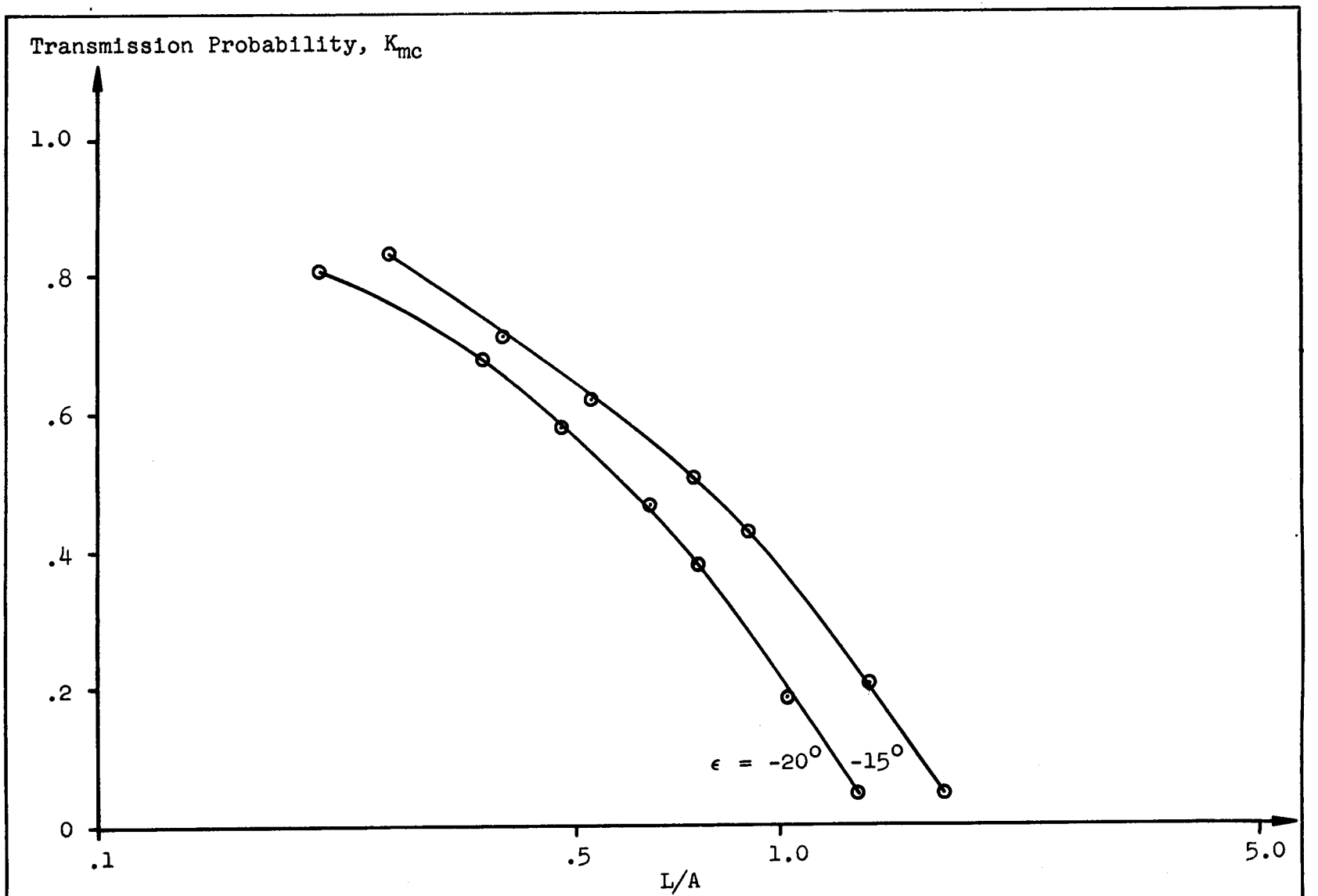

FIG. 8. TRANSMISSION PROBABILITIES, K_{mc}, FOR INFINITELY WIDE, CONVERGING FLAT PLATES FOR VARIOUS L/A VALUES.

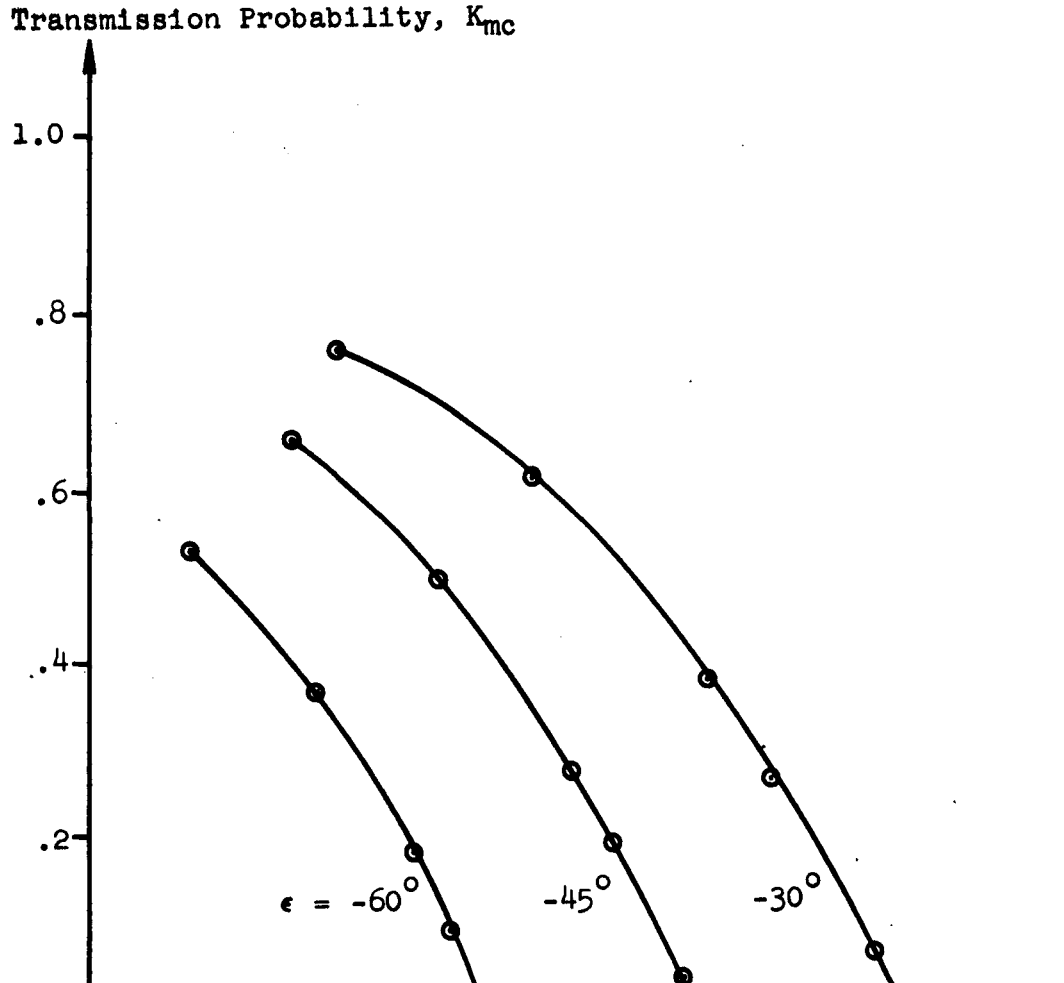

FIG. 9. TRANSMISSION PROBABILITIES, K_{mc},
FOR INFINITELY WIDE, CONVERGING FLAT PLATES FOR VARIOUS L/A VALUES

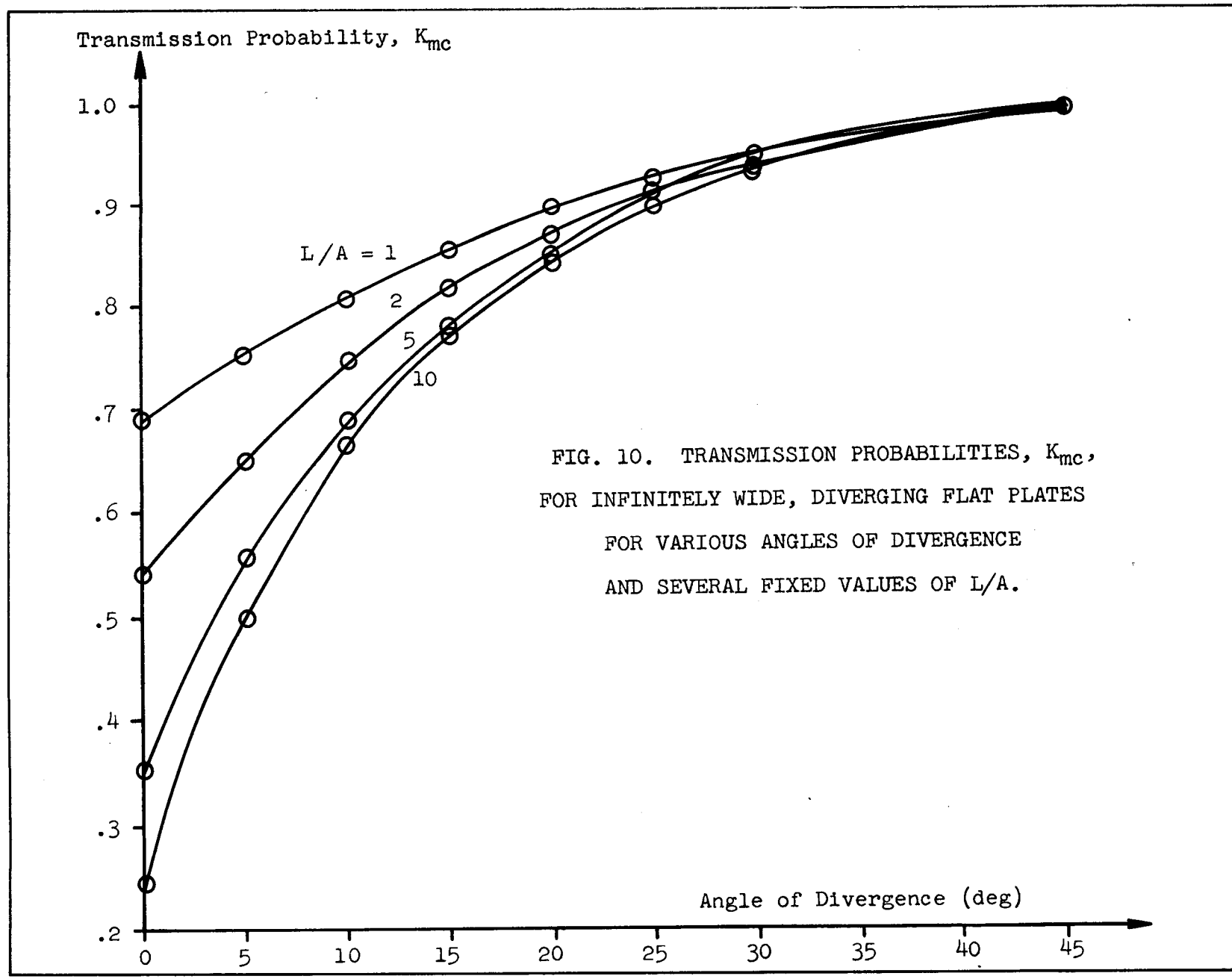

FIG. 10. TRANSMISSION PROBABILITIES, K_{mc}, FOR INFINITELY WIDE, DIVERGING FLAT PLATES FOR VARIOUS ANGLES OF DIVERGENCE AND SEVERAL FIXED VALUES OF L/A.

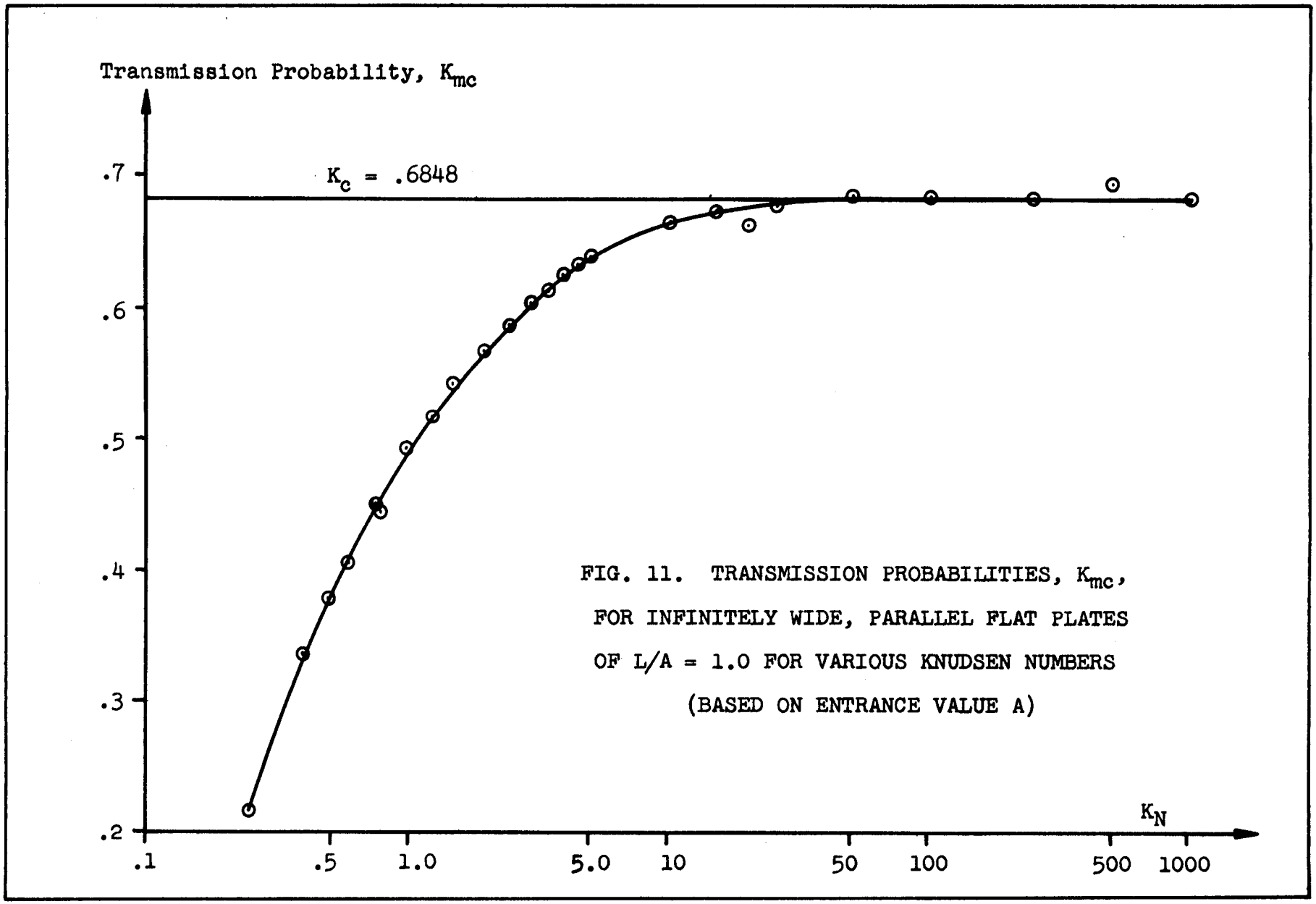

FIG. 11. TRANSMISSION PROBABILITIES, K_{mc}, FOR INFINITELY WIDE, PARALLEL FLAT PLATES OF L/A = 1.0 FOR VARIOUS KNUDSEN NUMBERS (BASED ON ENTRANCE VALUE A)

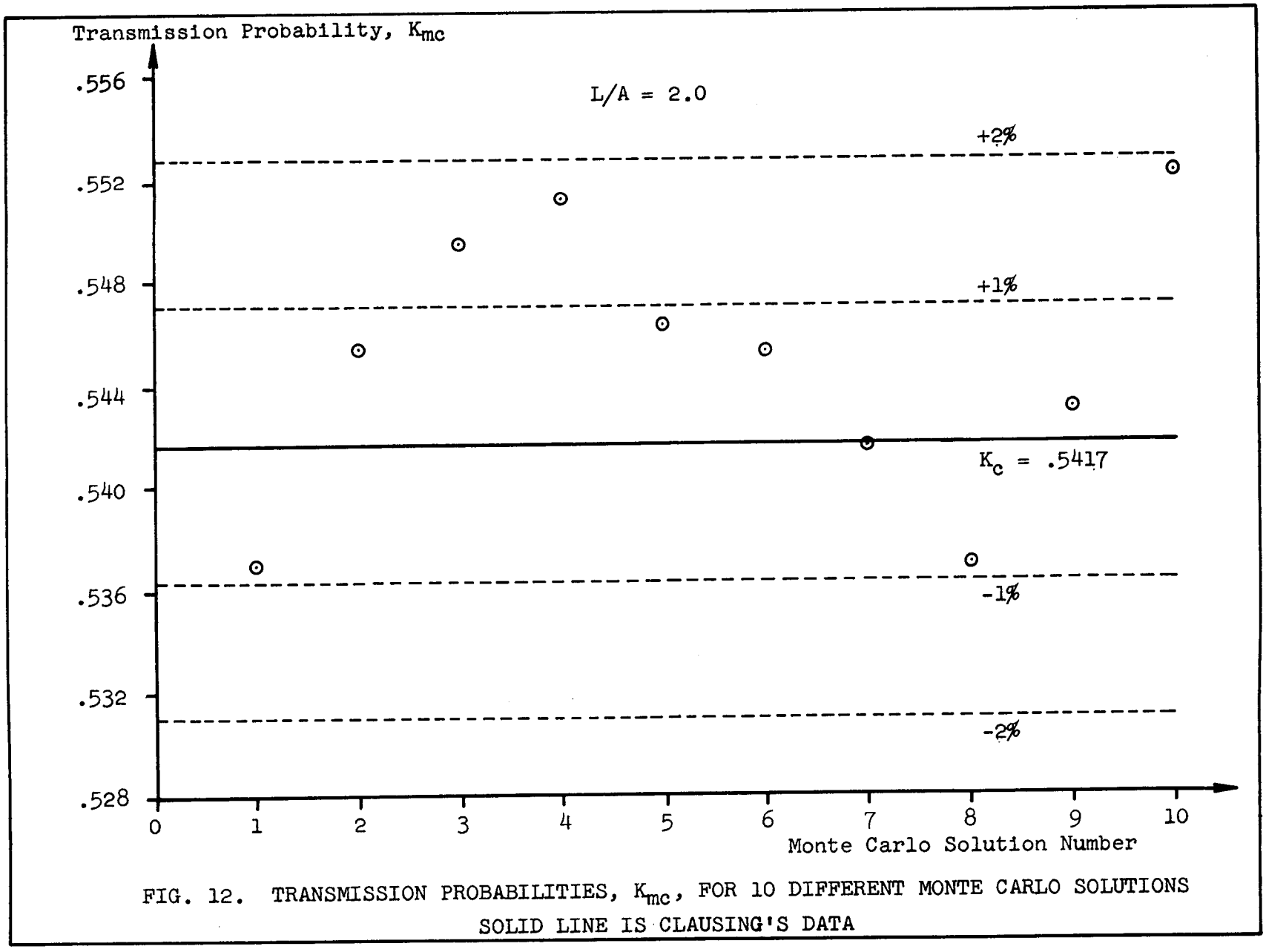

FIG. 12. TRANSMISSION PROBABILITIES, K_{mc}, FOR 10 DIFFERENT MONTE CARLO SOLUTIONS
SOLID LINE IS CLAUSING'S DATA

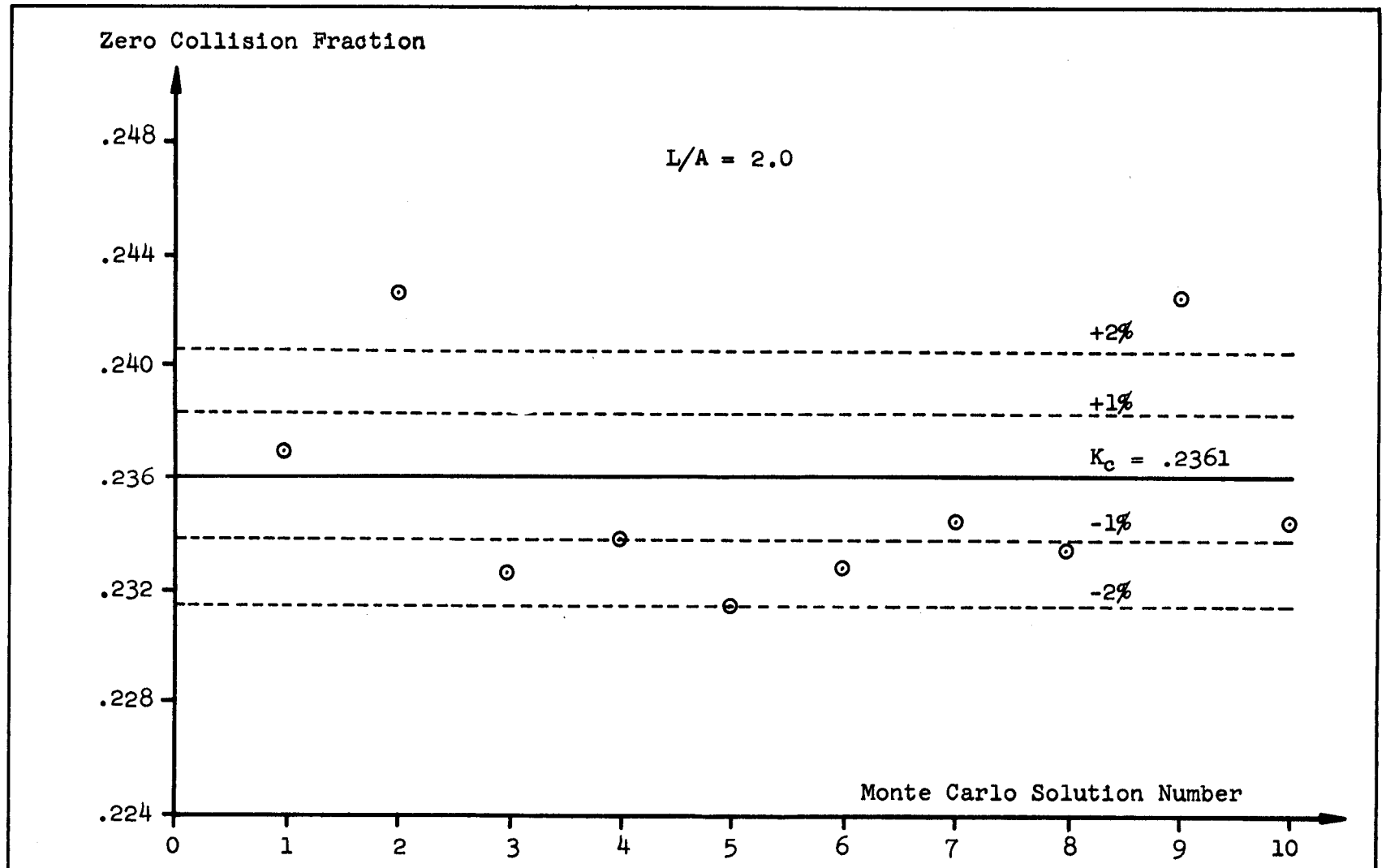

FIG. 13. FRACTION OF MOLECULES PASSING THROUGH THE SYSTEM WITHOUT COLLIDING WITH THE WALLS FOR TEN DIFFERENT MONTE CARLO SOLUTIONS

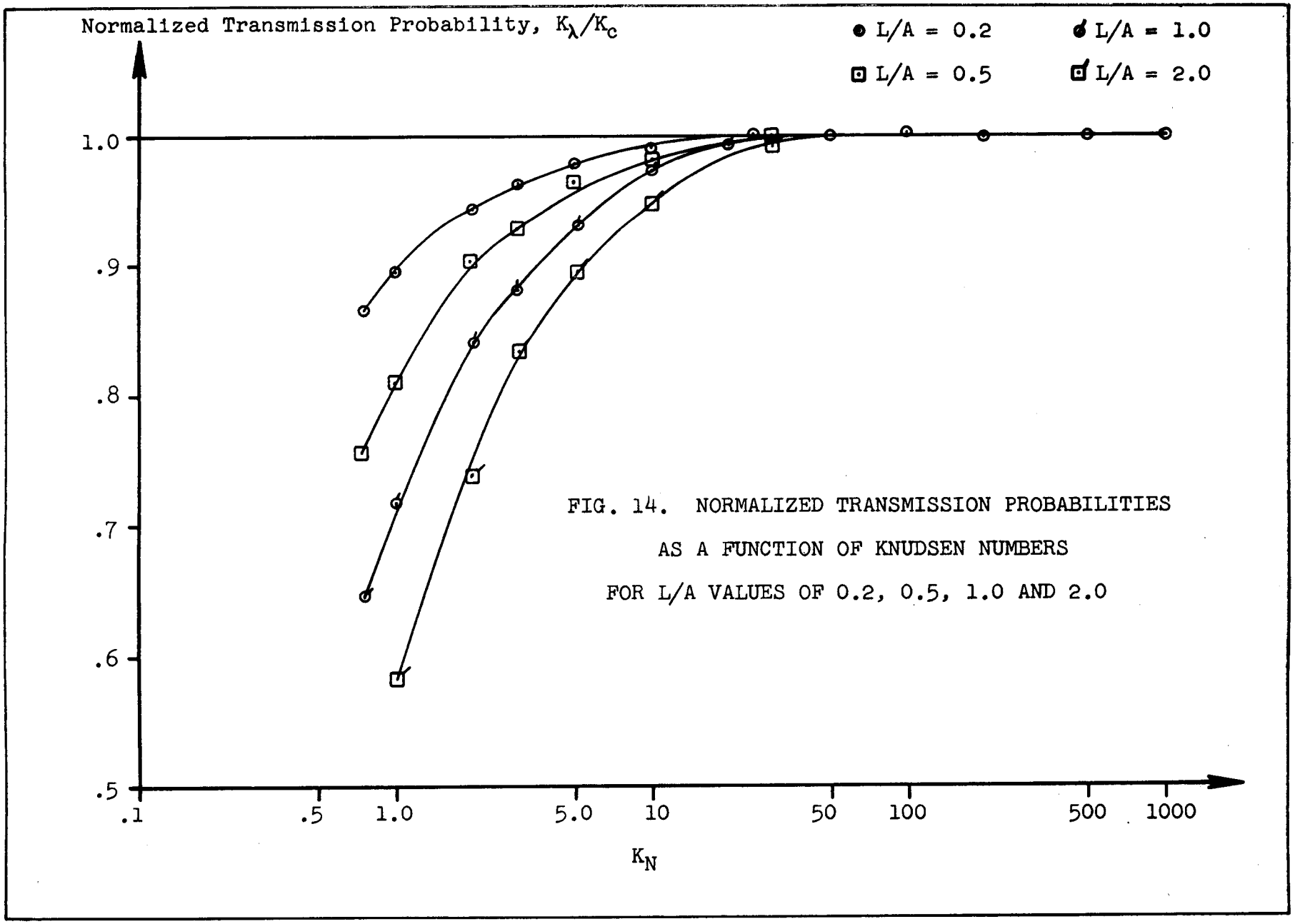

FIG. 14. NORMALIZED TRANSMISSION PROBABILITIES AS A FUNCTION OF KNUDSEN NUMBERS FOR L/A VALUES OF 0.2, 0.5, 1.0 AND 2.0

REFERENCES

1. Clausing, P., "Über die Strömung sehr verdunnter Gase durch Röhren von beliebiger Länge," Annalen der Physik, Vol. 5, pp. 961-989, 1932.

2. Davis, D. H., "Monte Carlo Calculation of Molecular Flow Rates Through a Cylindrical Elbow and Pipe of Other Shapes," Journal of Applied Physics, Vol. 31, p. 1169, July 1960.

3. Levenson, L. L., N. Milleron, and D. H. Davis, "Optimization of Molecular Flow Conditions," Vacuum Symposium Transaction (1960), p. 372, Pergamon Press, Oxford.

4. Ballance, J. O., W. K. Roberts, and D. W. Tarbell, "A Study of Cryo-pump Configuration in Free Molecular Flow Regions," Advances in Cryogenic Engineering, Vol. 8, K. D. Timmerhaus, editor, Plenon Press Inc., New York, 1963.

5. Tarbell, D. W. and J. O. Ballance, "A Study of the Distribution of Molecules Under Free Molecular Flow Conditions after Collisions with Simple Geometries," MTP-AERO-63-43, May 28, 1963, NASA, MSFC, Huntsville, Alabama, Unclassified.

6. DeMarcus, W. C. and F. H. Hooper, "Knudsen Flow Through a Circular Capillary," Journal of Chemical Physics, Vol. 23, p. 1344, July 1955.

APPROVAL NASA TM X-53112

MONTE CARLO SOLUTIONS OF KNUDSEN AND NEAR-KNUDSEN FLOW THROUGH INFINITELY WIDE, PARALLEL AND SKEWED, FLAT PLATES

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The information in this report has been reviewed for security classification. Review of any information concerning Department of Defense or Atomic Energy Commission programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.

This document has also been reviewed and approved for technical accuracy.

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