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Report 3866

COMPUTER SOLUTION OF SOME TRANSPORT PHENOMENA PROBLEMS

Joanna W. Schot

COMPUTATION AND MATHEMATICS DEPARTMENT
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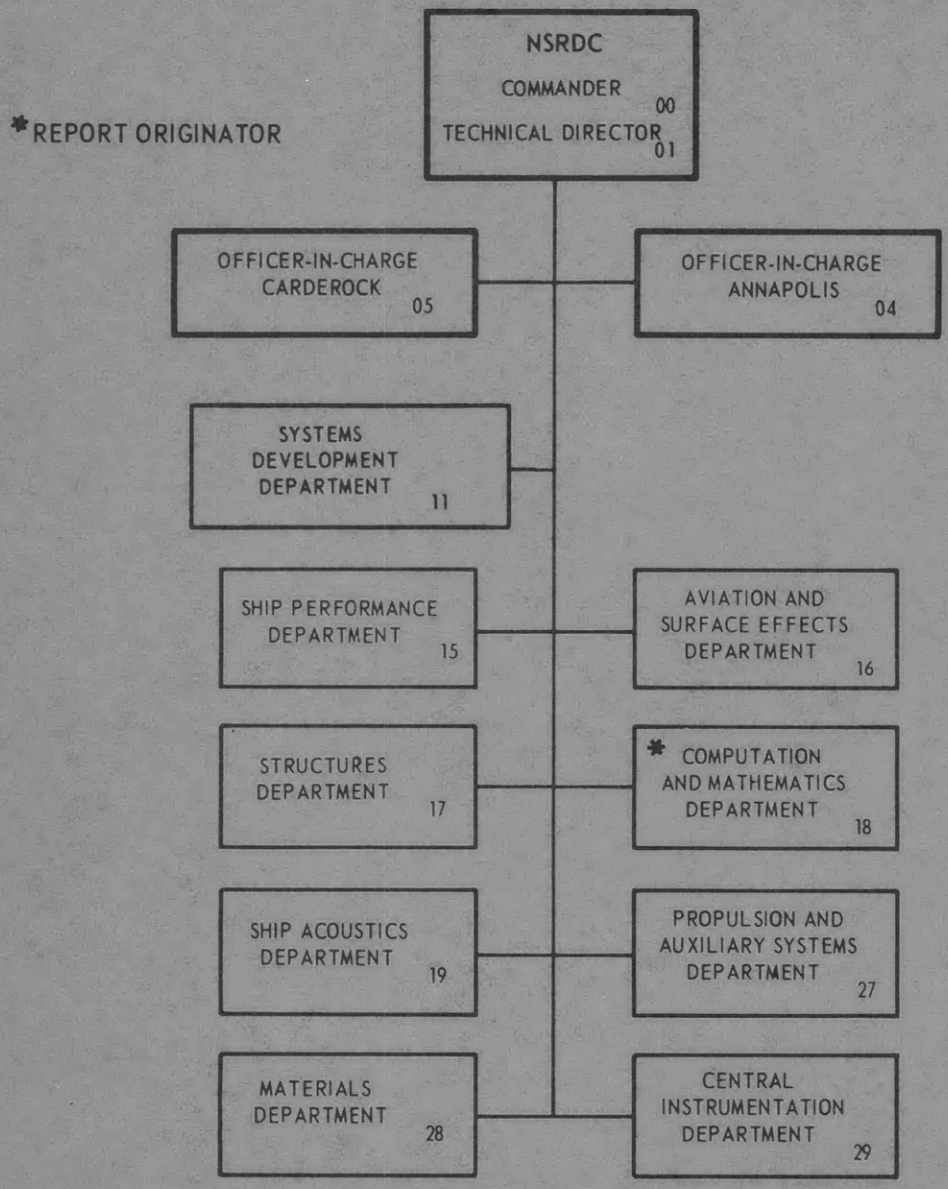

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by

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ABSTRACT

Advances in electronic computer methods for solving two specific types of three-dimensional boundary value problems are described. Early developments in calculating the diffusion of neutrons in nuclear reactors led to sophisticated computer programs for predicting the lifetime behavior of proposed reactor cores. One such program was developed in the 1960's to perform the time-dependent criticality calculations for intricate arrangements of fuel elements, control rods, and other components in three spatial dimensions. Up to 100,000 mesh points were permitted to adequately approximate the core geometry and material composition of the reactor. Normalized block iteration techniques were developed especially to handle the large coefficient matrices (up to 10^{10} entries) generated by the program. Secondly, experience gained with these reactor simulation programs, coupled with advances in computer technology, have made it possible to attack the very difficult nonlinear boundary value problems of viscous fluid motion. Several recently developed programs for studying rotating viscous fluids and the behavior of fluids moving past obstacles of different shapes are described briefly. Computer-generated pictures illustrating the phenomenon of vortex shedding are presented. These programs solve only fairly simple time-dependent viscous flow problems in two spatial dimensions (homogeneous, incompressible fluids, and simple geometric shapes), yet the solutions obtained for specific studies, such as rotating flow in a closed tank whose

cover rotates at a different rate from that of the fluid in the tank, have revealed unexpected flow phenomena. Problems associated with the solution of full-scale three-dimensional and time-dependent exterior flows are discussed. Physical insight already gained, plus expected advances in computers in the next five years, should permit the solution of practical viscous flow problems in three space dimensions plus time.

ADMINISTRATIVE INFORMATION

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COMPUTER SOLUTIONS OF SOME TRANSPORT PHENOMENA PROBLEMS

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INTRODUCTION

Electronic digital computers have been in existence for only a quarter of a century, a time span relatively short in the history of scientific achievement. Yet in this brief period computing technology has grown to such an extent that computers can now be used to numerically simulate complex physical processes, thereby providing scientists with a new approach to the investigation of unsolved problems in mathematical physics. This is possible because of the tremendous advances that have been made in the performance characteristics of computers, in the techniques of computer programming, and in the mathematical analysis of numerical methods [1], [2], [3].*

In this paper, we shall trace the increasing effectiveness of computer methods developed at the Naval Ship Research and Development Center for solving some boundary value problems dealing with transport phenomena. First, the solution of neutron diffusion problems as applied to the design of nuclear reactors will be discussed. Secondly, programs for studying the behavior of moving viscous fluids will be described. In both cases finite-difference methods are used. The physical process is mathematically formulated by an initial-boundary value problem defined over a specified region of space and time. A network or grid of points is superimposed on the region, and a system of difference equations is derived for each of the partial differential equations of the problem. To adequately model even linear boundary value problems, as in the

*References are listed on page 21.

diffusion of neutrons in reactor cores, this procedure may lead to systems of many thousands of equations in as many unknowns, whose solution requires sophisticated numerical methods. Even greater computational demands are made by the nonlinear problems of viscous flow at moderate Reynolds numbers.

NUCLEAR REACTOR SIMULATION

The success of computers in solving nuclear reactor problems is based on their ability to calculate rapidly and in intricate detail the physical changes occurring within the core of a reactor over a period of time. These changes induced by nuclear fission involve variations in the neutron population, the depletion of fuel, and the buildup and decay of fission products. The fact that the carriers of the chain reaction, namely the free neutrons in the core, are themselves produced by fission leads to an eigenvalue problem in which the eigenfunction represents the neutron flux distribution while the corresponding minimum eigenvalue is the criticality factor. When this factor is very close to unity, the chain reaction is self-sustaining, and the reactor is said to be critical.

One of the most successful early programs which solved steady-state reactor criticality problems was the Cuthill Code [4], [5] developed at NSRDC. This program mathematically modeled a two-dimensional cross section of a heterogeneous reactor composed of specified arrangements of diffusion and control regions. On the assumption that the neutron energy range could be divided into a fast and a slow energy group, the two-group diffusion theory approximation to the steady-state Boltzmann transport equation was used. Equations of the following form were solved in each diffusion region

$$\begin{cases} \operatorname{div}(D_s \operatorname{grad} \phi_s) - A_s\phi_s + B_f\phi_f = 0 \\ \operatorname{div}(D_f \operatorname{grad} \phi_f) - A_f\phi_f + \eta B_s\phi_s = 0 \end{cases},$$

where subscripts s and f refer to the fast and slow energy groups, respectively, $\phi(x,y)$ is the neutron flux, η is the eigenvalue which determines the criticality factor, $D(x,y)$ is the diffusion coefficient for the given diffusion region, $A(x,y)$ represents the total absorption coefficient, and $B(x,y)$ is a production coefficient. Certain boundary conditions must be satisfied along the interfaces between different materials as well as on the outer surface of the reactor. These equations were approximated by a system of finite-difference equations defined over a square network of points superimposed on a cross section of the reactor. Figure 1 illustrates one type of reactor configuration. The square grid used in the Cuthill Code is shown in Figure 2. Problems with 2,000 grid points were solved on the UNIVAC computer in 1956 in ten hours. This program, extremely limited by today's standards, provided good first approximations to the solution of the neutron diffusion problem. An example of a computer-generated plot of flux density contour lines for one problem is shown in Figure 3. A year later an improved version of the Cuthill Code was operational on the Naval Ordnance Research Calculator (NORC), a forerunner of the IBM 704 computer, and problems of similar size could then be solved in less than two hours.

The computing speeds and internal storage capacities of these machines were so limited [1], that considerable ingenuity was required to develop workable computing algorithms for reactor problems. These algorithms took advantage of the sparseness and non-negative properties of the coefficient matrices of the systems of difference equations [6], [7]. Many different mathematical and numerical techniques were developed to cover all aspects of reactor analysis, and by 1960 computers were well-established as important tools in reactor design [8], [9], [10]. Programs based on transport theory, such as the Thermal Energy Transport Codes by Dawson [11] were employed to determine the

angular dependence of the neutron flux in sensitive regions of the core. These programs produced numerical solutions to the steady-state Boltzmann equation on the NORC, UNIVAC-LARC, and the IBM 7090 computers with increasing speed and versatility.

The challenging problem of developing a very large time-dependent, three-dimensional reactor depletion program was solved when the FLAME code became operational on the UNIVAC-LARC in 1962 [12]. This highly flexible program simulated the lifetime behavior of heterogeneous water-moderated nuclear reactors by computing the neutron flux, the associated source, and the criticality factor at specified times, as well as the depletion of fuel and the buildup of fission products over specified intervals of time. The depletion calculations were based on the isotopic density method developed at the Westinghouse Atomic Power Laboratory [13]. The depletion equations comprised thirteen coupled first-order differential equations describing the growth and decay of the densities of the various isotopes constituting the composite material at each point (cell) in the reactor. These equations were used to calculate the changes in the reactor for a given time step based on the neutron flux distribution determined by the criticality calculations performed at the beginning of a time step.

To provide sufficient detail of the geometry and material composition of the reactor components (fuel elements, moderator, reflector, control rods, etc.) up to 100,000 grid points and several hundred material compositions could be handled by FLAME for a two-group problem. Seven-point difference equations were used to approximate each of the group equations. (Up to four groups were permitted.) This resulted in a system of 100,000 linear equations for each energy group. The full coefficient matrices, therefore, would contain up to 10^{10} entries. Fortunately, these matrices were sparse, with at most seven non-zero elements per row, and they were set up in such a way that normalized

block iteration [7] was used to solve the equations. This is a method developed from the well-known successive overrelaxation method [14], and its use increases the rate of convergence of the iteration process. Since the solution of the group equations was the most time-consuming part of the program, accelerating the convergence was extremely important. A set of reports completely documents the mathematical and programming techniques used [15]. Even though the FLAME program taxed the storage capacity of the LARC, by tailoring the numerical methods and data-handling techniques to take advantage of the LARC's special features*, the lifetime histories of many proposed reactor designs were simulated in a few hours. For example, one time step of a 50,000-point, four-group problem was solved in 1½ hours. When compared with the ten hours required to solve the more restricted 2,000-point problem on the UNIVAC only six years earlier, these figures illustrate the growth rate in the effectiveness of computers in solving reactor problems. (See Table I.) Power predictions based on reactor calculations agreed within 1 to 2 percent with measured values of reactors performing at full power. Moreover, reactor depletion studies led to design improvements that significantly increased the lifetime of power-producing nuclear reactor cores. The reactor simulation methods summarized here were used by naval reactor contractors** to develop production codes for use in their reactor design projects.

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* The LARC was one of the first dual processing computers, permitting many functions to be performed simultaneously.

** Westinghouse Atomic Power Division, Westinghouse Electric Corporation and Knolls Atomic Power Laboratory, General Electric Corporation.

TABLE I - TIME REQUIRED TO SOLVE SELECTED PROBLEMS ON DIFFERENT COMPUTERS

PROBLEM	PROGRAM	GEOMETRY AND SIZE OF PROBLEM	COMPUTER, DATE & MEMORY SIZE	RUNNING TIME IN MINUTES
Neutron diffusion, 2 groups	Cuthill	(x, y) 2,000 points	UNIVAC; 1956 (1,000 words)	600
	NORC-Cuthill	(x, y) 2,000 points	NORC; 1957 (2,000 words)	120
Fuel depletion, 4 groups	FLAME	(x, y, z, t) 50,000 points	UNIVAC-LARC; 1962 (3,030,000 words)	90 per time step
Neutron transport, 39 groups, 70 regions	TET	(x, u, μ) slab geometry	IBM 7090; 1964 (32,000 words)	5 to 45
Viscous flow past arbitrary body	DMC	(x, y, t); 2500 points, 600 time steps	IBM 360/91; 1970	135
Viscous flow past angled elliptic plate	ROPE	(η, θ, t); 6,000 points, 2,000 time steps	IBM 360/91; 1971	60 per shedding cycle
Viscous flow in rotating tank	ROTA	(r, ϕ, z, t); 1681 points, 2,000 time steps	IBM 360/91; 1971	15

VISCOUS FLOW SIMULATION

The solution of the mathematical and numerical problems associated with reactor simulation suggested the use of similar computer methods to attack the nonlinear boundary value problems of viscous flow. Moreover, powerful computing systems such as the IBM 360/91 and the CDC 6700 plus the automatic plotting capability afforded by the Stromberg-Carlson 4020 Microfilm Recorder made it feasible to simulate certain simple viscous flow situations and represent the computed results visually. To demonstrate what has already been achieved, several recently developed programs are currently being used to study in detail the flow properties near highly curved body surfaces, across induction slots, and the intriguing behavior of rotating fluids. One of these programs is the Dawson-Marcus Code (DMC), which calculates laminar incompressible flow about arbitrarily shaped two-dimensional bodies [16]. This program solves the vorticity-stream function formulation of the Navier-Stokes equations and uses special outer boundary conditions to account for the finite size of the flow field. The basic differential equations are

$$\Delta\psi = -\omega$$

$$\frac{\partial\omega}{\partial t} = -\frac{\partial}{\partial x}\left(\omega\frac{\partial\psi}{\partial y}\right) + \frac{\partial}{\partial y}\left(\omega\frac{\partial\omega}{\partial x}\right) + \frac{1}{Re}\Delta\omega ,$$

where Δ is the Laplacian operator, $\psi = \psi(x, y, t)$ is the stream function, $\omega = \omega(x, y, t)$ is the vorticity, (x, y) are the rectangular spatial coordinates, t is the time, and Re is the Reynolds number defined by $Re = LU/\nu$. Here L is the maximum diameter of the body, U is the free stream velocity and ν is the kinematic viscosity of the fluid.

Using specially developed finite-difference approximations over a grid of about 5,000 points, the program permits the body to be specified

by a discrete set of boundary points. This is to provide for the study of flows past bodies which do not fit into a natural coordinate grid system. Vorticity, i.e., the angular velocity of a fluid element, is the crucial quantity which characterizes the flow disturbances created by the presence of an obstacle in the flow field [17]. To calculate vorticity in the immediate neighborhood of the body, a special regridding scheme is used in DMC to increase the number of grid points close to the body surface, as shown in Figure 4. The entire flow region calculated is about 10 times as wide and 20 times as long as the diameter of the body. The program was tested for the case of flow past a circular cylinder at low Reynolds numbers, using 20 points to specify the boundary of the cylinder. About 600 time steps were required to reach a periodic solution for the problem with a Reynolds number of 100. The total elapsed computer time on the IBM 360/91 was $2\frac{1}{4}$ hours, including the calculation of streamlines and vorticity lines for plotting time-sequence pictures on the microfilm recorder. A computer-generated motion picture of these results was made which illustrates the phenomenon of vortex shedding. A few frames from this film are shown in Figure 5.

Numerical studies of flows around flat plates are more difficult and require much more computer time than circular cylinders because of the high surface curvature at the ends of the plates [18], [19]. Lugt and Haussling [20] have carried out a numerical study of the characteristics of vortex shedding from slender elliptically shaped plates at various angles of inclination. Their computer program makes use of an elliptic coordinate system (η, θ) with the surface of the plate located at $\eta = \eta_0$. The vorticity-stream function equations are solved by finite-difference techniques using the Gauss-Seidel line over-relaxation method for the Poisson equation. The Dufort-Frankel method is used to compute the change in vorticity with advancing time. The

flow is impulsively started from an initial potential flow solution. For the case of a slender plate $\eta_0 = 0.1$ inclined at an angle $\alpha = 45^o$ and Re = 200, a sequence of plots of streamlines and vorticity lines is shown in Figure 6. The first cycle in the development of a Kármán vortex street is exhibited. When the body starts moving, a vortex develops immediately and separates from the trailing edge. This vortex is visible in the first (upper, left) picture as a wave in the streamlines. At the same time a vortex is generated behind the leading edge and is finally shed. Thus, the program simulates the production and shedding of vortices alternately from the two edges of the plate. Recent water tank photographs made by Honji verify these results [21].

About 6,000 spatial points and 2,000 time steps were required to obtain these results. Even though the flow region is homogeneous and the coefficient matrices do not have to be recomputed for each time step, as was the case for the heterogeneous reactor problems, the nonlinearity of the viscous problems creates additional computational requirements. In fact, attempts to solve the problem of a rotating elliptic plate indicated that present iteration methods would require a prohibitive amount of computer time. However, a direct method for solving the Poisson difference equations, such as the cyclic block reduction method [22], [23] can reduce the time required to solve certain problems by a factor of as much as 15.

Another computer study of viscous flow behavior was made of circulation patterns in rotating tanks, where the covers revolve at different angular speeds [24]. From the initial solid-body rotation a meridional and an azimuthal circulation relative to the moving tank develop. No finite gap between tank and cover is assumed, and the singular behavior at this interface is investigated. The problem is formulated as a laminar axisymmetric flow of an incompressible fluid in a circular-

cylindrical tank of radius L and height H, which is spinning with the constant angular velocity Ω. Cylindrical polar coordinates (r, ϕ, z) are used together with the corresponding velocity components (u, v, w) in a reference frame which rotates with the tank. Initially, the cover impulsively starts to rotate with the constant angular velocity $\Omega_c \neq \Omega$. The characteristic numbers used in comparing different rotational flows are the Rossby number, defined by $Ro = (\Omega - \Omega_c)/\Omega$, and the Ekman number, defined by $Ek = \nu/(\Omega H^2)$, where ν is the kinematic viscosity. A sequence of pictures at various times showing the transient stage for $Ek = 0.001$ are presented in Figure 7. Two time periods are clearly distinguishable: the spin-up time and the time necessary for the flow to reach near steady-state. These pictures are frames from a computer-generated motion picture which shows the development of secondary circulations from the initial solid-body rotation. Unexpected and heretofore unknown flow phenomena in the transient phase were revealed; namely, cells in the meridional circulation and counter currents in the azimuthal direction appear and vanish before the steady-state is reached.

These examples of viscous flow analysis using computer methods indicate that numerical experiments may be carried out on computers to study fluid flow phenomena that cannot be readily isolated in physical experiments. The study of vorticity dynamics is greatly aided by controlled computer experiments, whereas only crude measurements of vorticity can be obtained in wind or water tunnels [25]. The ease with which hypothetical flow situations may be modeled using programs such as those described in this paper excites the imagination of fluid dynamicists. Recently, considerable interest in slip flow has instigated computer studies on the generation and propagation of vorticity in flows past bodies under the perfect-slip boundary condition [26]. Flow separation,

instability, and vortex-shedding still occur under this hypothetical condition, i.e., that the shear stress is zero on the surface of the body. Anticipated improvements in computers over the next five years coupled with the development of new numerical methods should lead to more general computer studies of viscous flows in three spatial dimensions at higher Reynolds numbers. Even though it is unlikely that turbulent flows can be directly simulated by these methods, the fact remains that computers show great promise in advancing the understanding of fundamental flow phenomena.

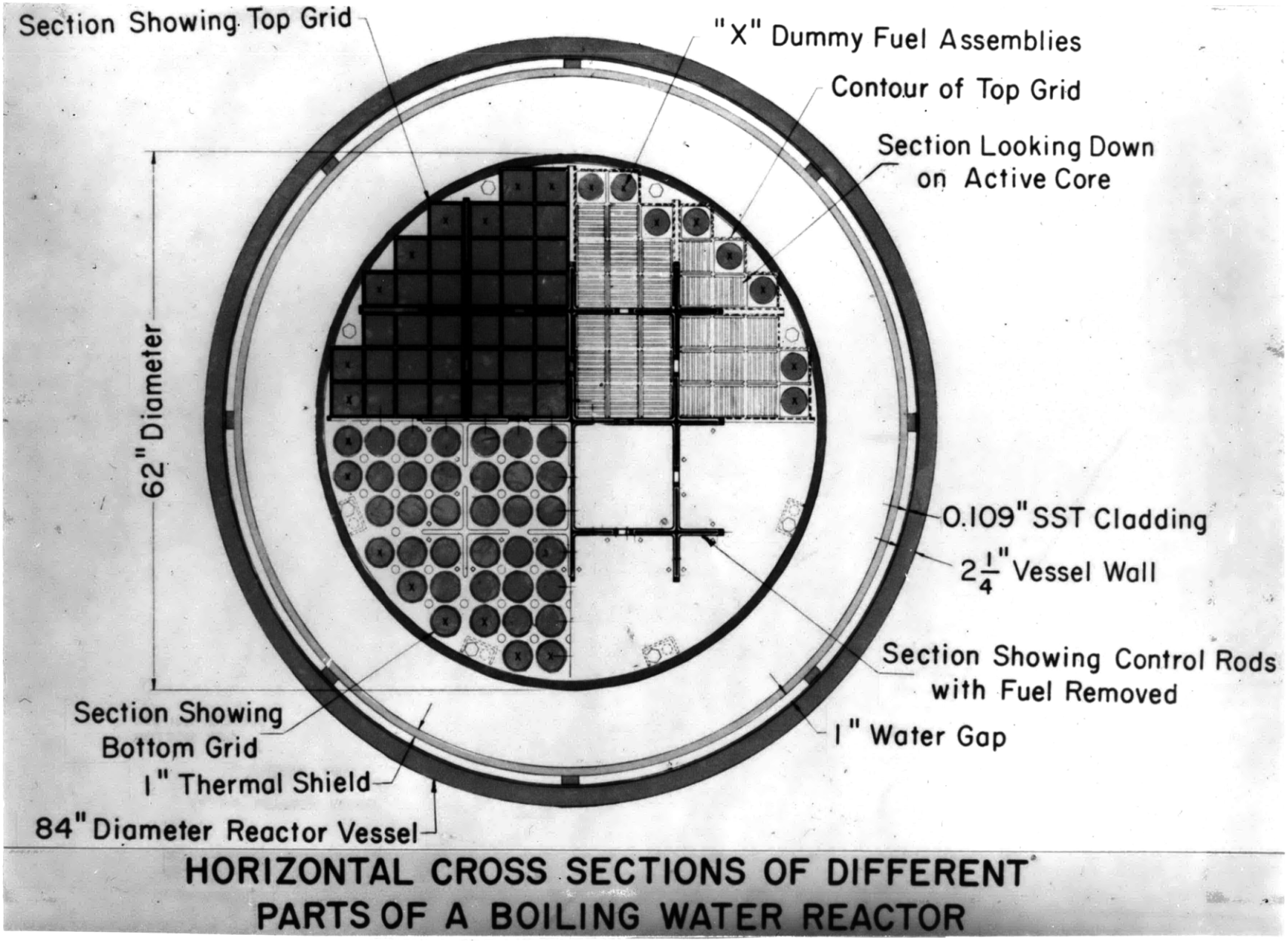

Figure 1 - One type of reactor configuration

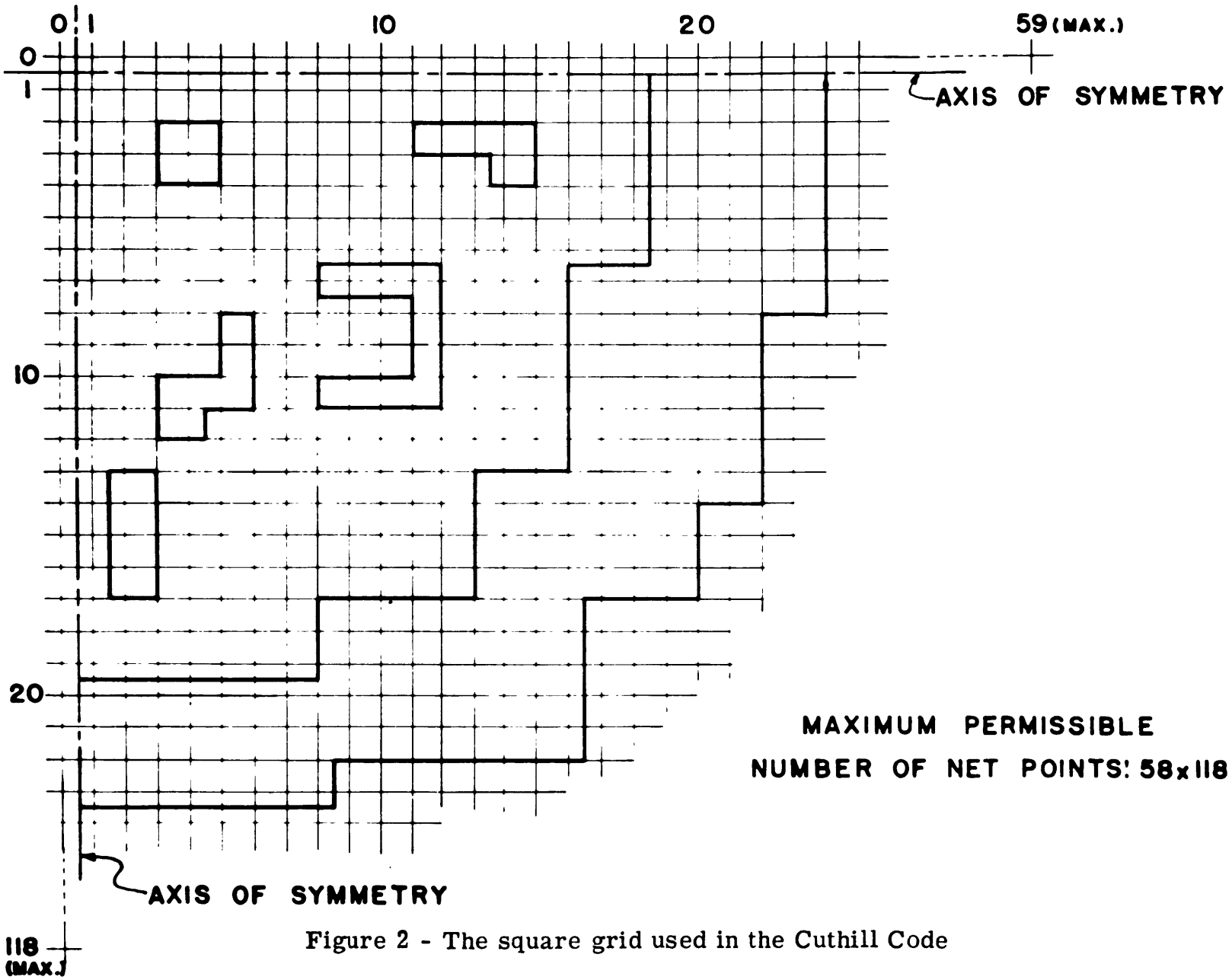

Figure 2 - The square grid used in the Cuthill Code

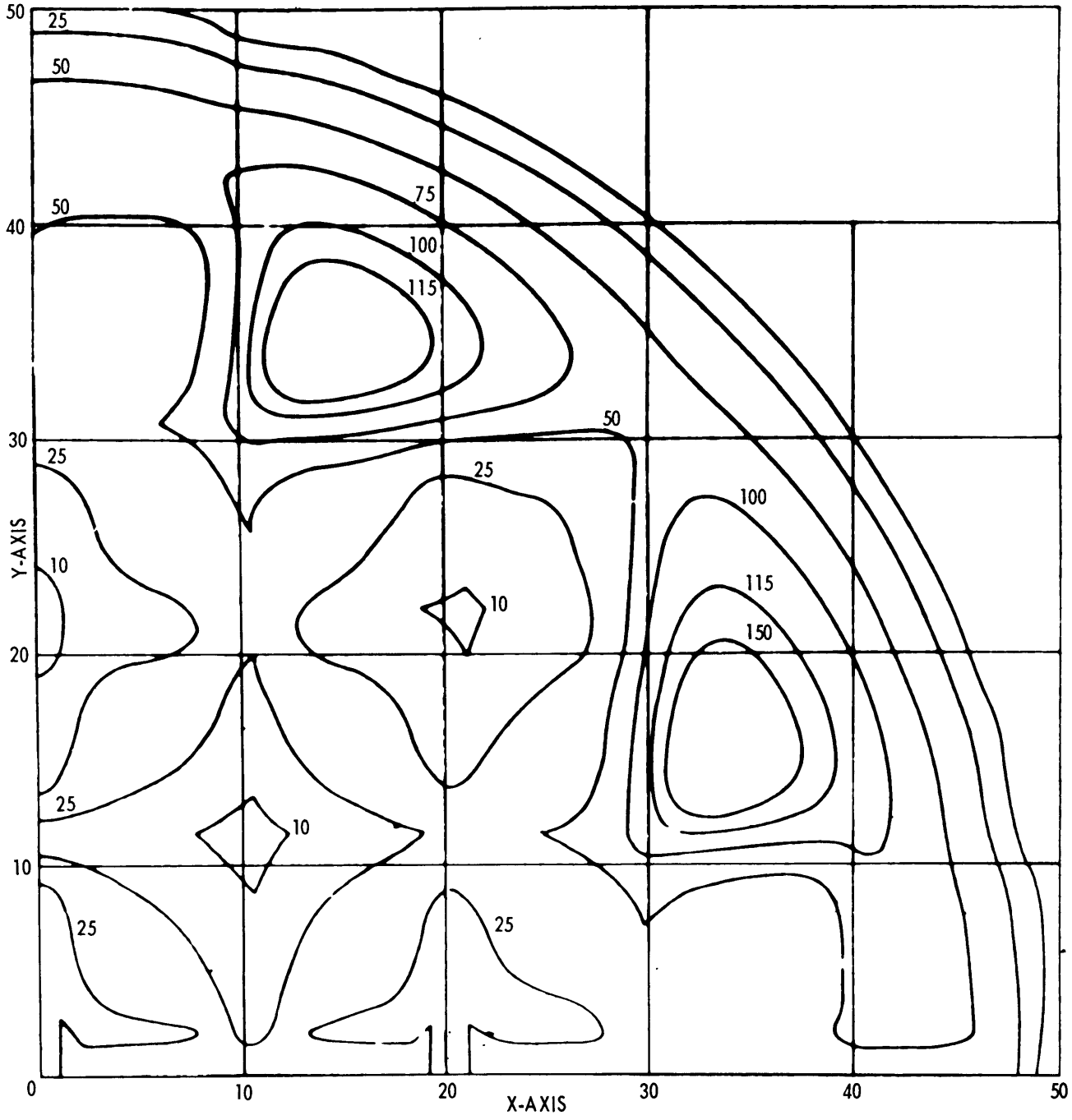

Figure 3 - Computer-generated flux density contour lines

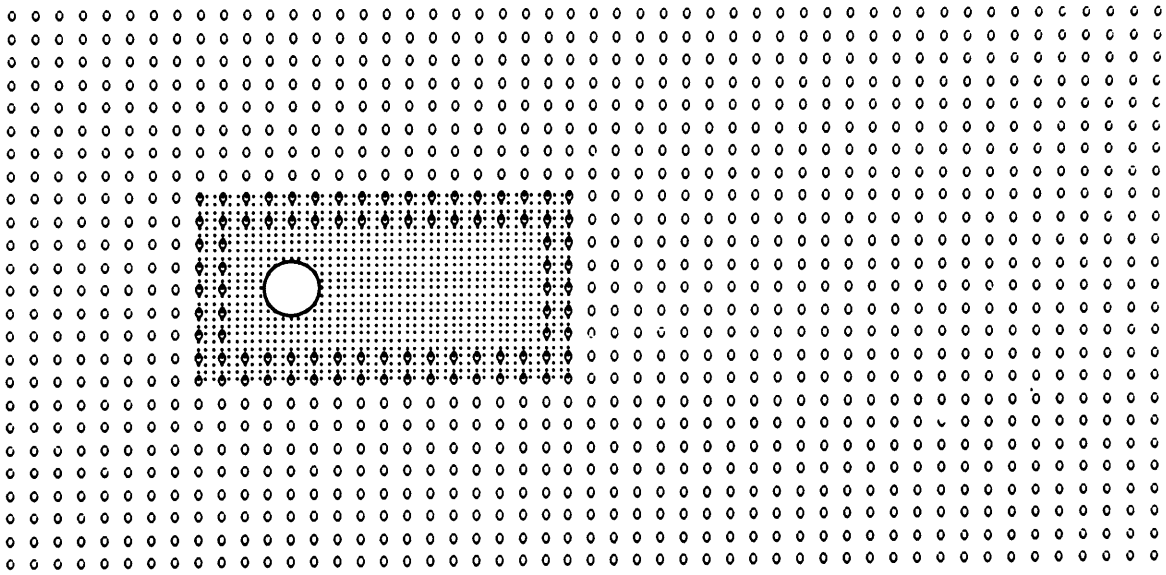

Figure 4 - The flow field grid scheme used in DMC

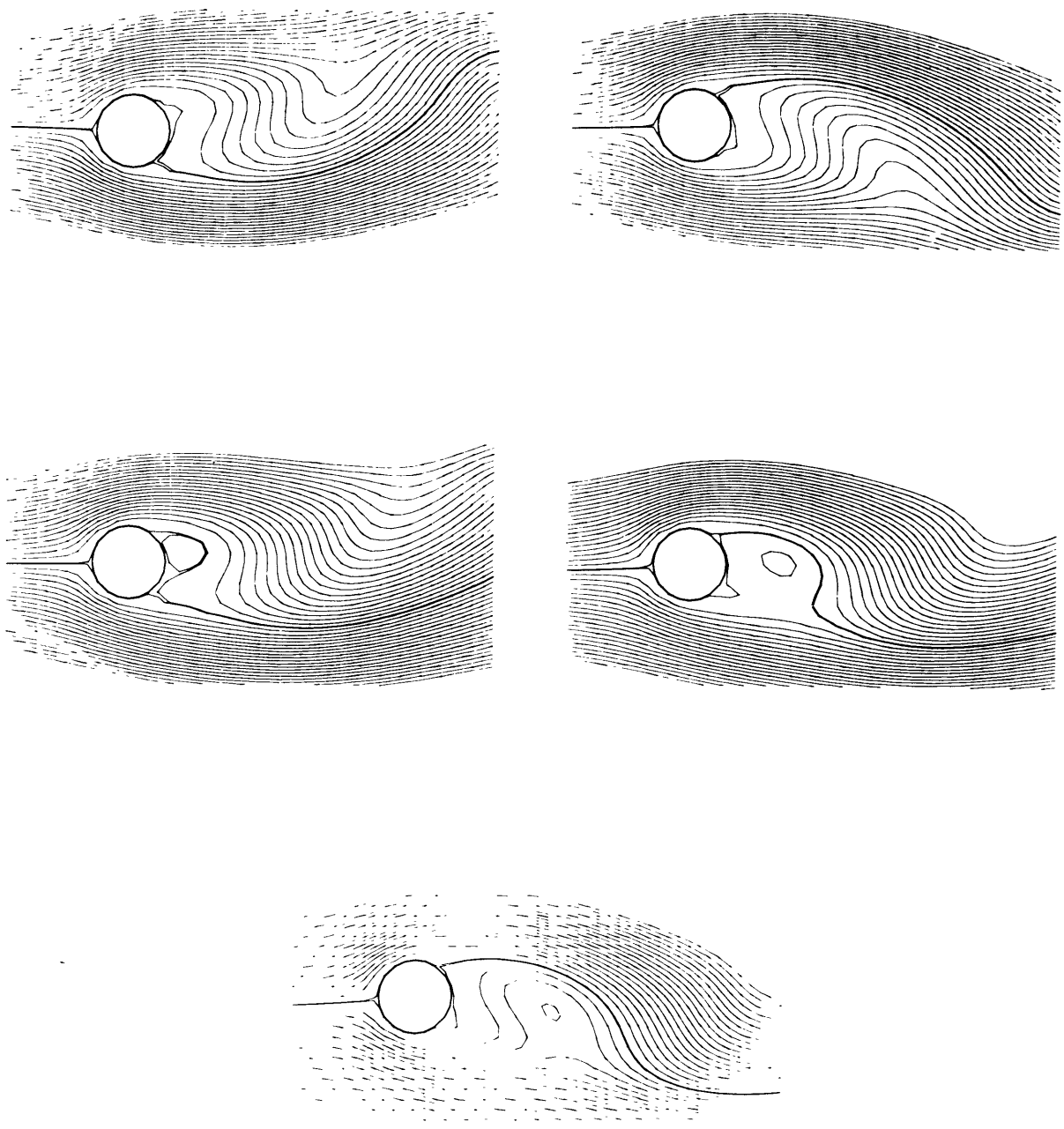

Figure 5 - Streamlines showing vorticity shedding at Re = 100

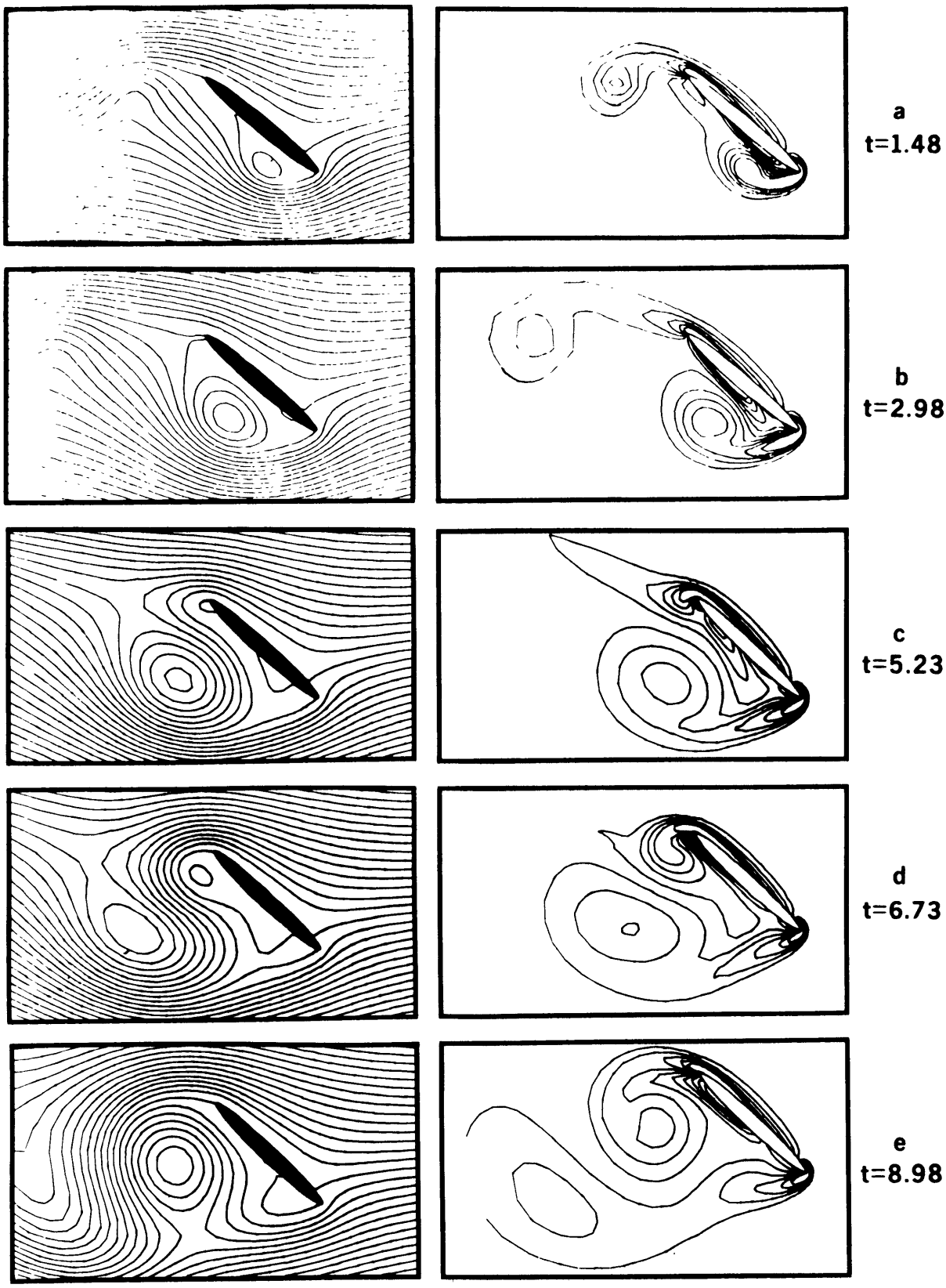

Figure 6 - Sequence of streamlines and equal-vorticity lines for Re = 200, $\alpha = 45^{o}$, $\eta_0 = 0.1$. (Flow direction is from the right.)

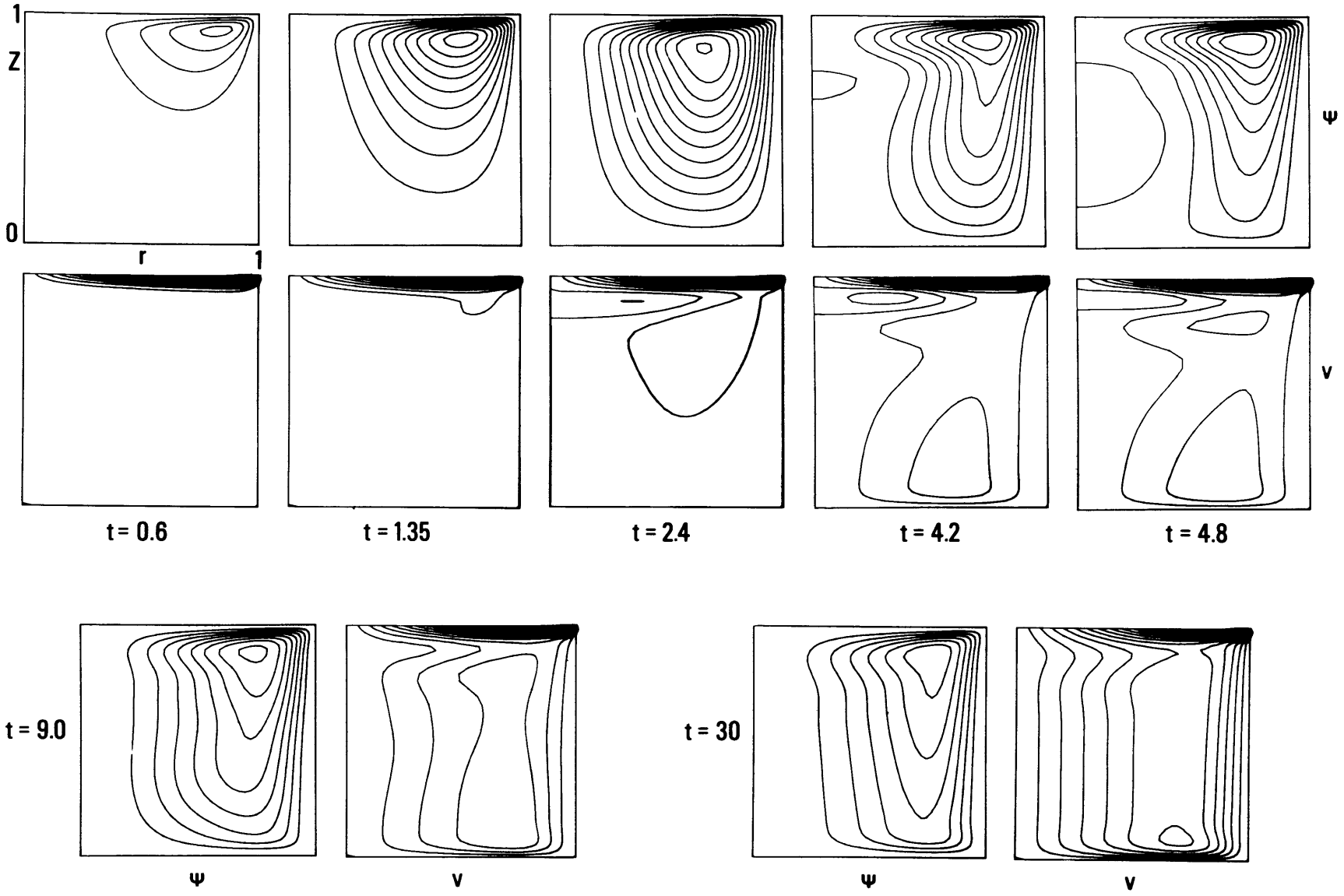

Figure 7 - Lines of constant ψ and v at various times for a tank rotating about the z-axis. The rotation of the cover has been stopped abruptly at t=0. Ro = 1, H/L = 1.

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13 ABSTRACT

Advances in electronic computer methods for solving two specific types of three-dimensional boundary value problems are described. Early developments in calculating the diffusion of neutrons in nuclear reactors led to sophisticated computer programs for predicting the lifetime behavior of proposed reactor cores. One such program was developed in the 1960's to perform the time-dependent criticalifty calculations for intricate arrangements of fuel elements, control rods, and other components in three spatial dimensions. Up to 100,000 mesh points were permited to adequately approximate the core geometry and material composition of the reactor. Normalized block iteration techniques were developed especially to handle the large coefficient matrices (up to 10^{10} entries) generated by the program. Secondly, experience gained with these reactor simulation programs, coupled with advances in computer technology, have made it possible to attack the very difficult nonlinear boundary value problems of viscous fluid motion. Several recently developed programs for studying rotating viscous fluids and the behavior of fluids moving past obstacles of different shapes are described briefly. Computer-generated motion pictures illustrating the phenomenon of vortex shedding are presented. These programs solve only fairly simple time-dependent viscous flow problems in two spatial dimensions (homogeneous, incompressible fluids, and simple geometric shapes), yet the solutions obtained for specific studies, such as rotating flow in a closed tank whose cover rotates at a different rate from that of the fluid in the tank, have revealed unexpected flow phenomena. Problems associated with the solution of full-scale three dimensional and time-dependent exterior flows are discussed. Physical insight already gained, plus expected advances in computers in the next five years, should permit the solution of practical viscous flow problems in three-space dimensions plus time.

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