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NUMERICAL SIMULATION OF NATURAL CONVECTION IN A SPHERICAL CONTAINER DUE TO COOLING AT THE CENTER (IDEALIZATION OF THE LAL/KROES EXPERIMENT)

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FOREWORD

This document reports the results of effort by personnel of Lockheed Missiles & Space Company, Inc., Huntsville Research & Engineering Center, for the National Aeronautics and Space Administration under Contract NASW-3281, "Manufacturing in Space: Fluid Dynamics Numerical Analysis." The NASA Technical Director is Dr. Robert F. Dressler, Manager, Advanced Technology Program, NASA Headquarters, Washington, D.C.

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ABSTRACT

Natural convection in a spherical container with cooling at the center was numerically simulated using the Lockheed-developed General Interpolants Method (GIM) numerical fluid dynamics computer program. The numerical analysis was simplified by assuming axisymmetric flow in the spherical container, with the symmetry axis being a sphere diagonal parallel to the gravity vector. This axisymmetric spherical geometry was intended as an idealization of the proposed Lal/Kroes crystal growing experiment to be performed on board Spacelab. Results were obtained for a range of Rayleigh numbers from 25 to 10,000. For a temperature difference of 10 C from the cooling sting at the center to the container surface, and a gravitational loading of 10^{-6} g_e, a computed maximum fluid velocity of about 2.4×10^{-5} cm/sec was reached after about 250 sec. The computed velocities were found to be approximately proportional to the Rayleigh number over the range of Rayleigh numbers investigated.

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NOMENCLATURE

Symbol	Description
g	gravity force in units of acceleration
g_e	gravitational acceleration on surface of earth, 980 cm/sec^2
r	radial distance
R	sphere radius
Ra	Rayleigh number = $\dfrac{g\beta \, \Delta T \, R^3}{\nu\alpha}$
T	temperature
ΔT	temperature difference between cooled crystal growing surface at center of container and container wall
t	time
$\tilde{t}$	dimensionless time = $\nu t/R^2$
v	velocity
$\tilde{v}$	dimensionless velocity = $\dfrac{\nu}{g\beta \, \Delta T \, R^2} \, v$
α	thermal diffusivity
β	volumetric coefficient of thermal expansion
ν	kinematic viscosity
ψ	stream function

v

INTRODUCTION

One of the proposed experiments to be performed using the Fluids Experiment System (FES) facility aboard Spacelab is the Lal/Kroes experiment (Ref. 1), which is concerned with the controlled growth of a single crystal under near-zero gravity conditions. The crystal is to be grown from a triglycine sulfate (TGS) solution contained in a 10 x 10 x 10 cm cubical shaped container. The concentration is to be nominally 45 g TGS/100 cc water. The temperature of the solution will be within the range of 35 to 50 C. The crystal will be grown on a cooled 1 cm diameter disk positioned at the center of the container at the end of a 2 cm diameter insulated sting. The disk will be cooled up to 10 C less than the surrounding container walls.

The purpose of the experiment is to study crystal growth in the absence of significant gravity induced convective stirring of the solution. The near elimination of convective stirring is expected to result in the growth of high quality crystals. The purpose of this numerical study is to predict the intensity of convective stirring due to the small residual gravity forces remaining under orbital flight conditions. The Lockheed developed General Interpolant Method (GIM) code computer program (Ref. 2) was used in the numerical simulations. This computer code numerically integrates the basic fluid dynamics equations in conservation form. Computations were performed on the NASA-Langley Cyber 203.

NUMERICAL SIMULATION

To permit reasonable economy in computer usage, the cubical shaped experiment configuration was modeled by a sphere of the same volume as the cubical container, with axisymmetric flow assumed. The axis of symmetry is along a sphere diameter parallel to the gravity vector. The nodal point distribution was generated by the GIM code geometry module by specifying an array of 20 x 10 area elements and 21 x 11 nodal points over the half-sphere cross section enclosed by a semicircular arc and sphere axis of symmetry. The geometry module treated the semicircular region as a four-sided figure, with the bottom side the axis of symmetry and the other three sides concentric circular arcs. The region was divided into an array of quadrilateral elements with curvilinear sides, and with the nodal points located at the corners of the individual elements. The geometry is shown in Fig. 1 with the computational grid network superimposed. The cooled crystal growing surface is represented by the outline of grid lines at the center of the sphere. The gravity vector is directed downward as shown in the figure.

A steady state conduction temperature distribution is generated by the computer program as an initial condition. The nodal points outlining the cooled crystal growing surface are maintained at a temperature 10 C less than the surrounding container surface.

The physical properties of the TGS solution were not well known at the time of this analysis. Based on conversations with Dr. R. L. Kroes, the NASA Principal Investigator, physical property values were assumed as listed in Table 1.
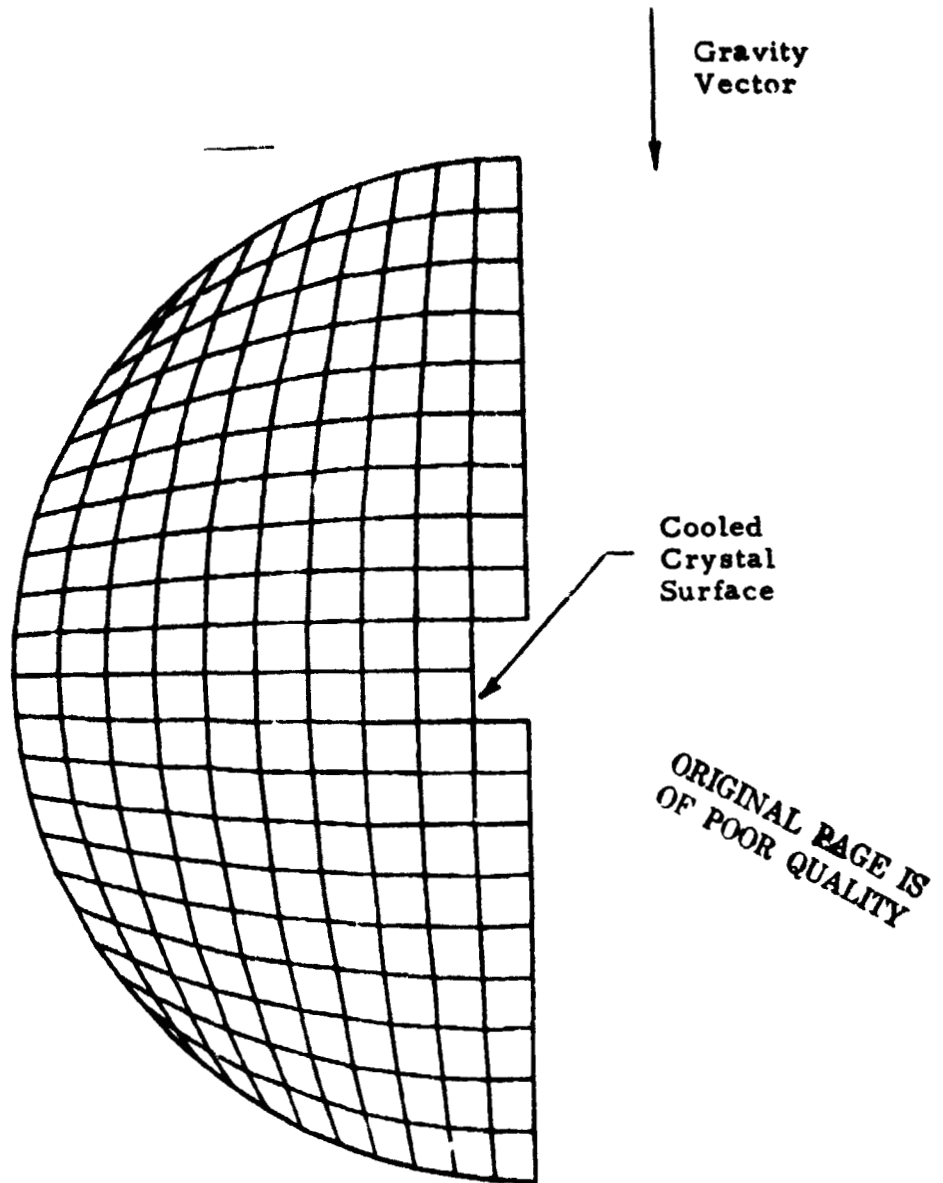
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Fig. 1 - Geometry and Computational Grid for Lal/Kroes Experiment Numerical Simulation

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Table 1

LIST OF ASSUMED PHYSICAL PROPERTY VALUES FOR TRIGLYCINE
SULPHATE (TGS) SOLUTION (45 g TGS/100 cc WATER)

Viscosity, μ	1.78 centipoise
Thermal Conductivity, k	0.00143 cal/cm-sec-C
Density, ρ	1.15 g/cm^3
Specific Heat, C_p	1.0 cal/gm-C
Thermal Expansion Coefficient, β	2.07 x 10^{-4}/C

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RESULTS

Numerical simulations were performed for Rayleigh numbers, Ra, vary-
ing from 25 up to 10,000. The computed spatial maximum velocities are plotted
in Fig. 2 as a function of time for the various Rayleigh numbers. Note that by
nondimensionalizing the velocity and time as shown, the results collapse very
closely about a single curve for Rayleigh numbers through 2500. The Ra =
10,000 results are in accord with the other Rayleigh number results through
the initial transient up to a dimensionless time of about 0.1.

For the lower Rayleigh numbers, the results shown in Fig. 2 indicate the
following approximate relationship for the spatial maximum velocity as a func-
tion of time·

$$v_{max} = 0.00485 \frac{g\beta \, \Delta T \, R^2}{\nu} \left[1 - \exp(-42 \frac{\nu t}{R^2}) \right]$$

$$\leq 0.00485 \frac{\alpha}{R} Ra \left[1 - \exp(-42 \frac{\nu t}{R^2}) \right]$$

For the Lal/Kroes experiment configuration, the equal volume sphere radius,
R, corresponding to the 10 x 10 x 10 cm cube is 6.2 cm. The time required to
reach steady state is about 250 sec after imposition of an impulse gravitational
load. The maximum spatial velocity at steady state is 2.4×10^{-5} cm/sec for
a 10^{-6} g_e gravitational load and a 10 C ΔT.

The temperature, streamline and velocity contours at steady state are
shown in Figs. 3 through 5 for various Rayleigh numbers. Note that the tem-
perature contour distortion from the conduction profile increases with
Rayleigh number as expected. The higher Rayleigh number temperature
contours show a strong distortion from the low Rayleigh number results. The
streamline contours, however, are basically unchanged over the range of
Rayleigh numbers, except for a relatively slight asymmetry introduced at
the higher Rayleigh numbers. The flow pattern consists of a single con-
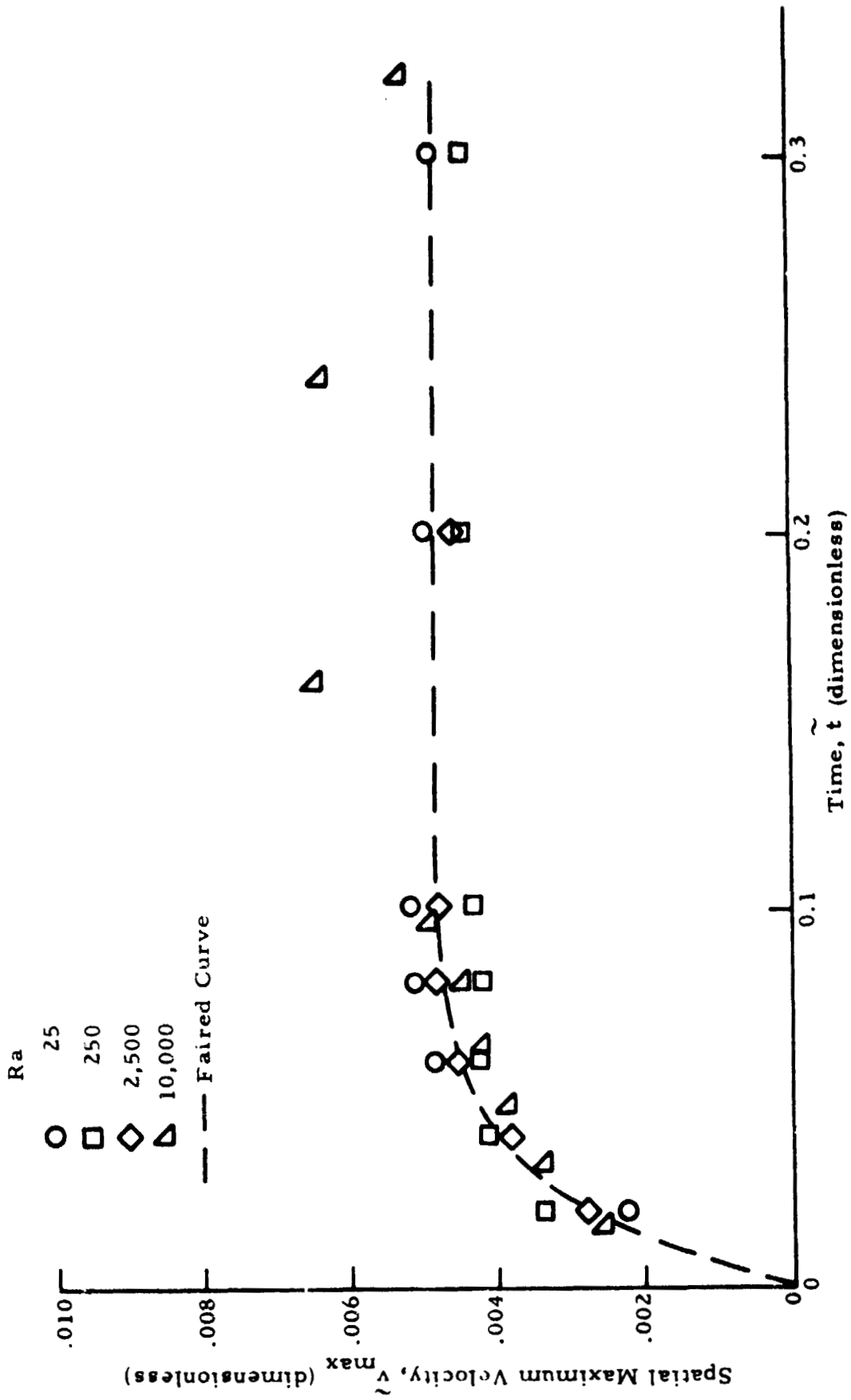vection cell for all of the Rayleigh numbers shown.

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Fig. 2 - Computed Spatial Maximum Velocity History for Idealized Lal/Kroes Experiment for Various Rayleigh Numbers
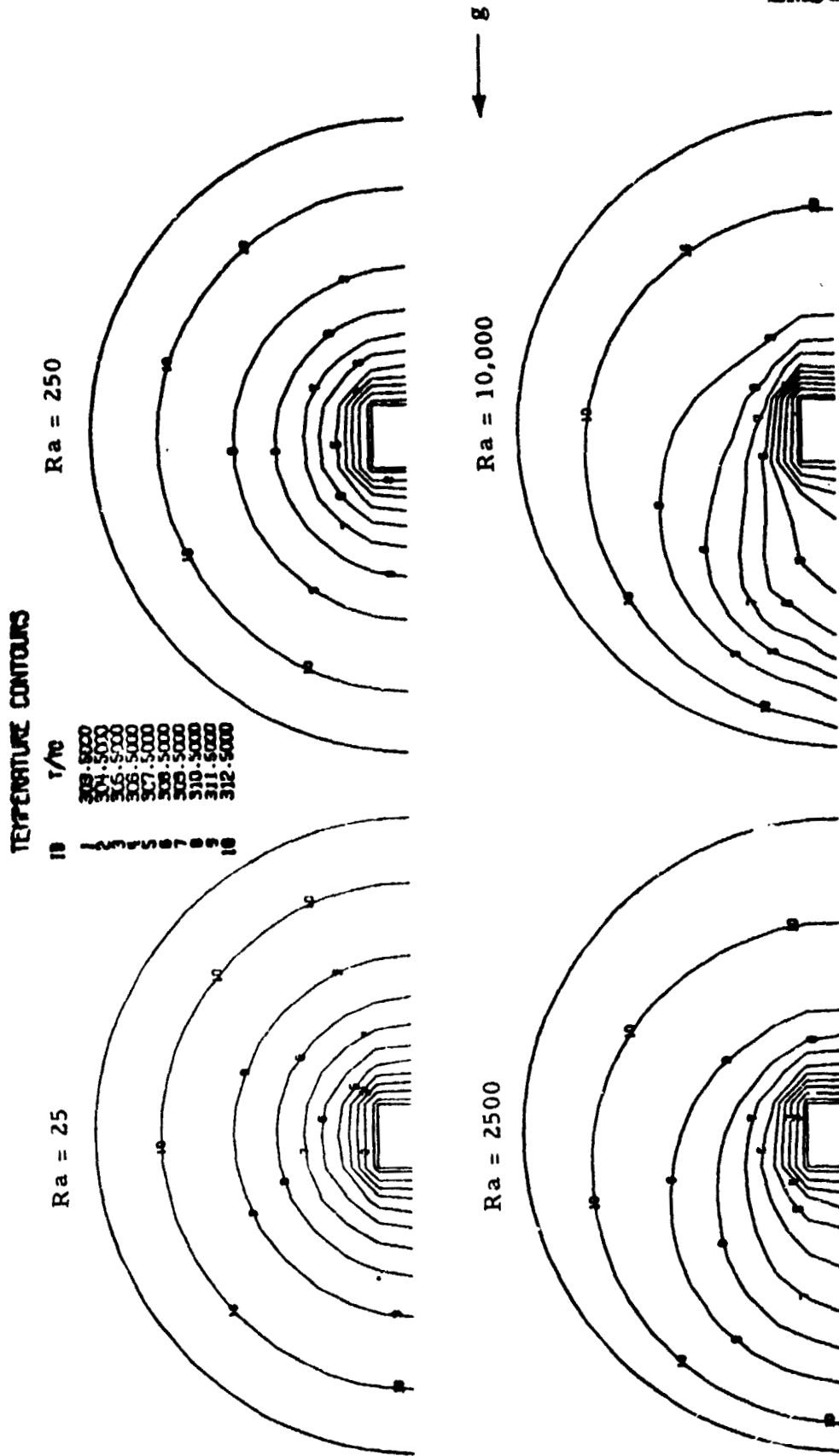
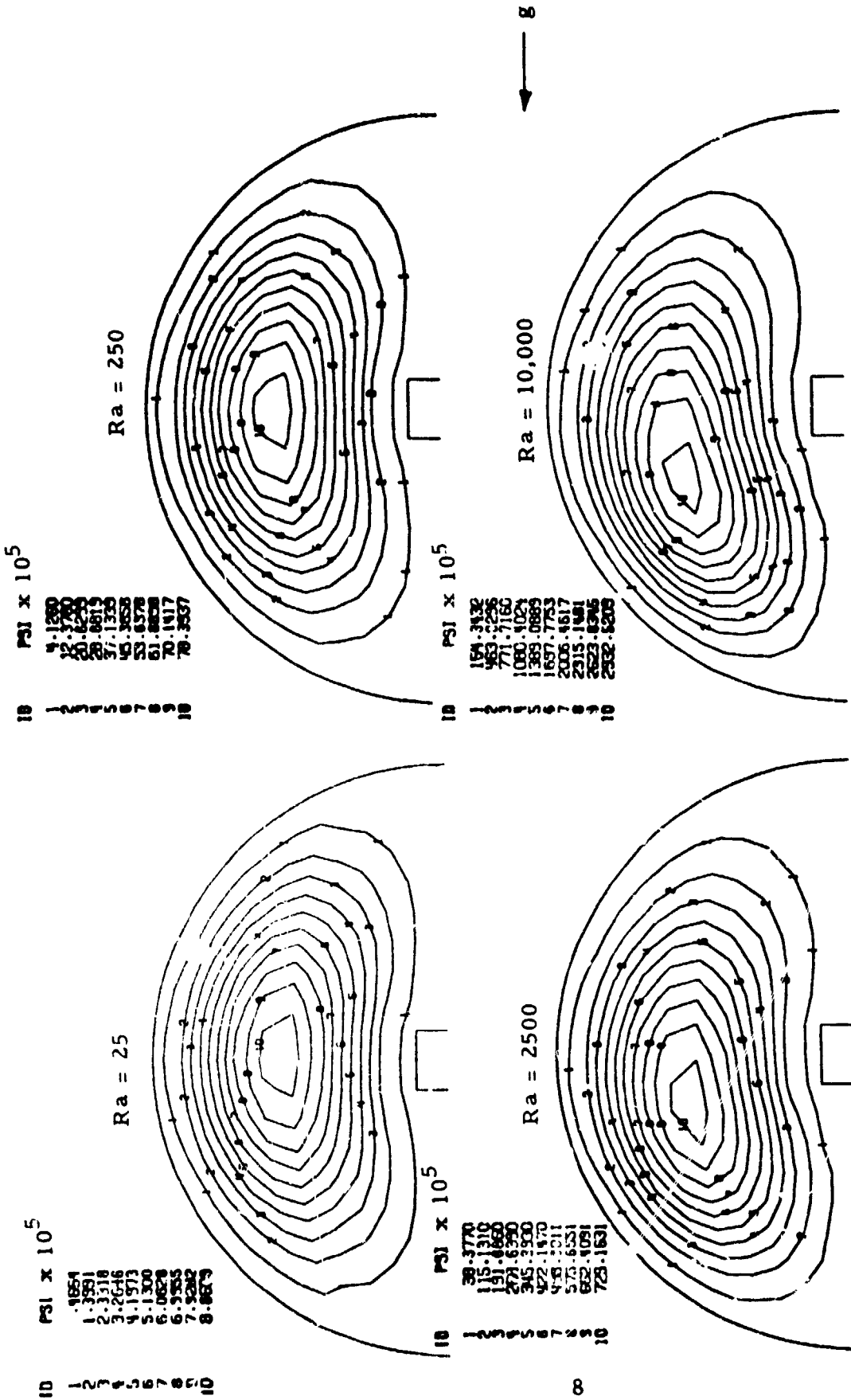Fig. 3 - Temperature Contours at Steady State for Various Rayleigh Numbers
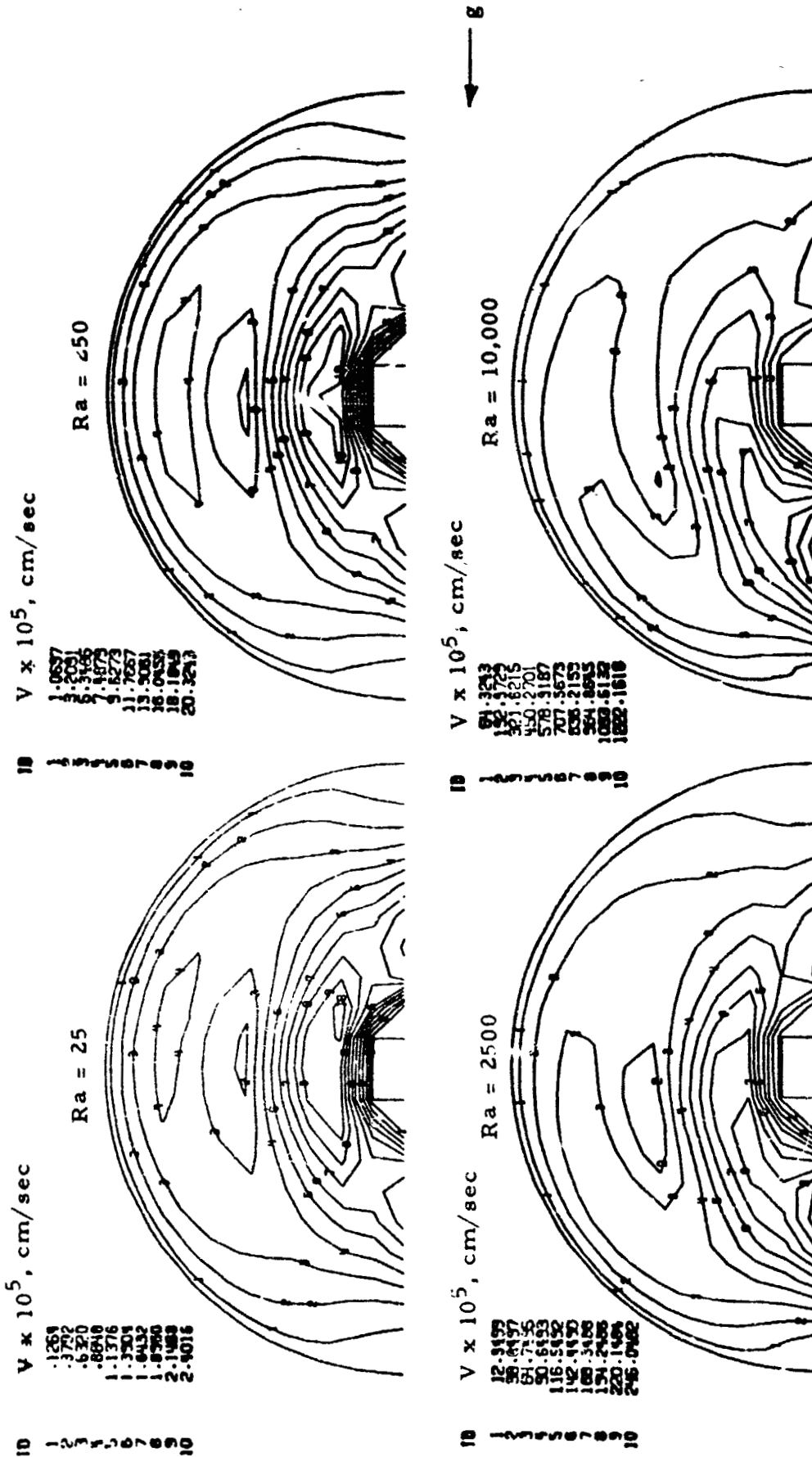
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Fig. 4 - Streamline Contours at Steady State for Various Rayleigh Numbers

Fig. 5 - Velocity Contours at Steady State for Various Rayleigh Numbers

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The variations in temperature, streamline and velocity contours with time are shown in Figs. 6, 7 and 8 for Ra = 10,000. As expected, the distortion in the temperature field increases with time toward the steady state condition. The single convection cell is also shown to shift gradually from the symmetry characteristic of low Rayleigh numbers toward the asymmetry characteristic of high Rayleigh numbers.
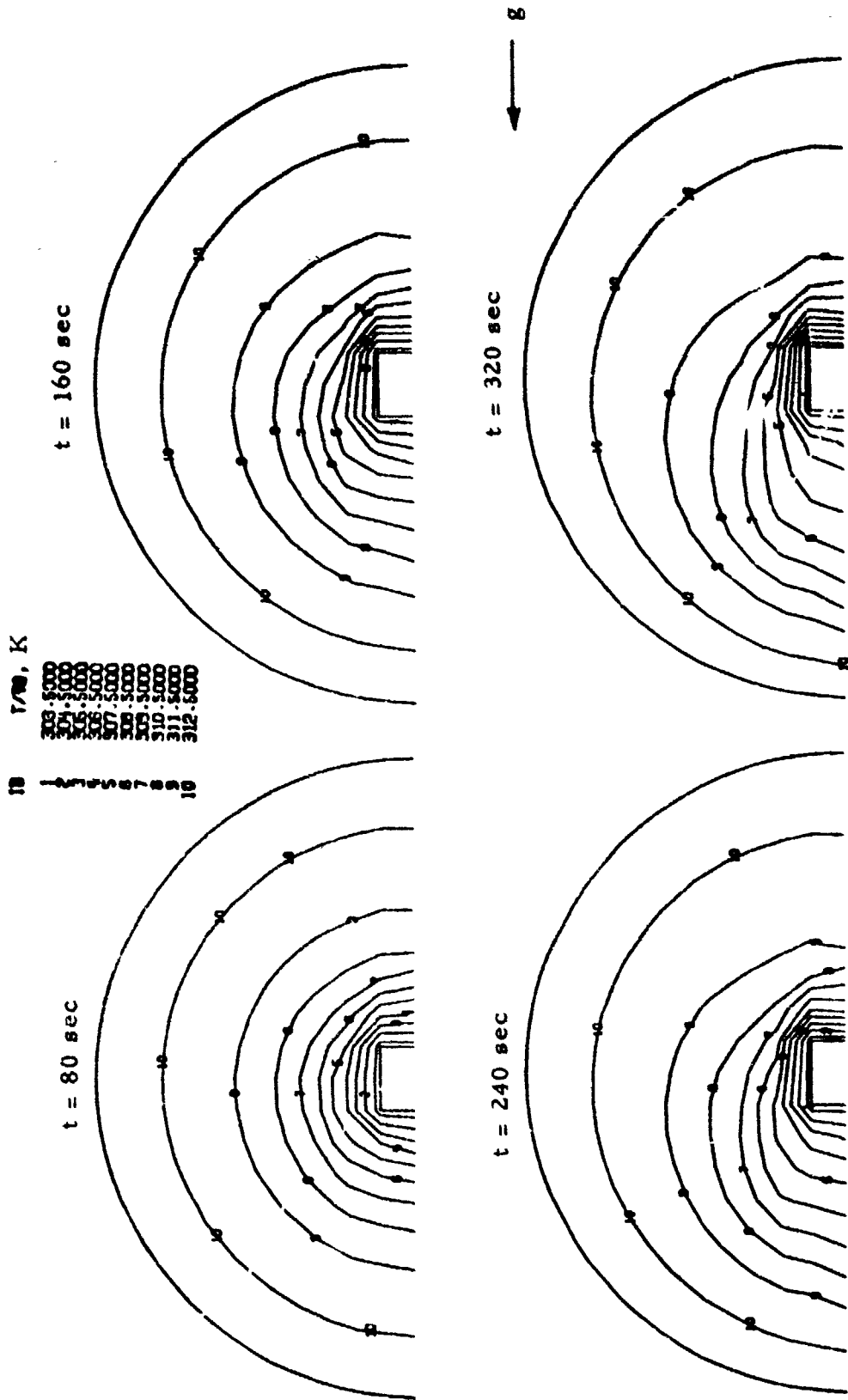
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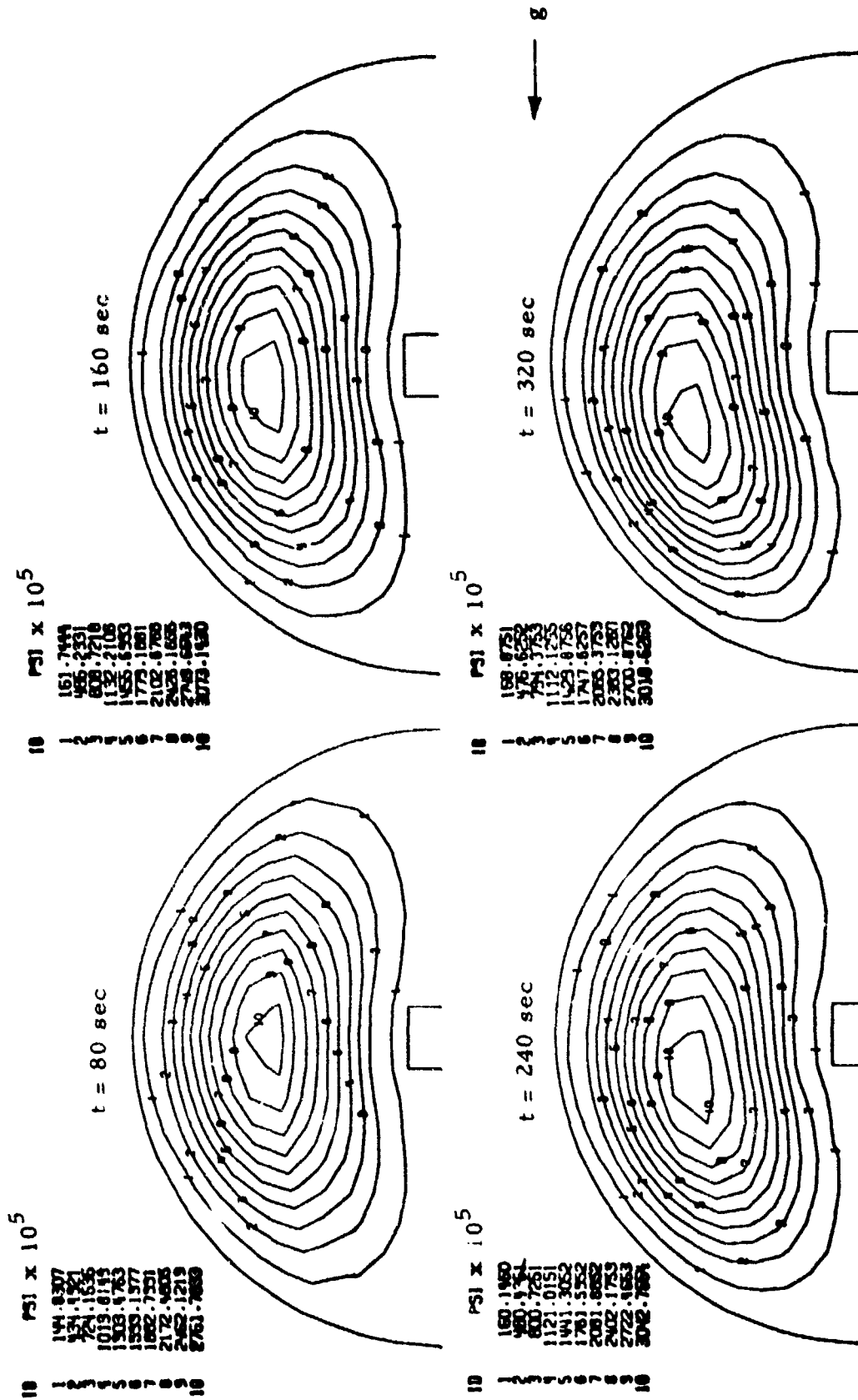Fig. 6 - Temperature Contours at Various Times for Ra = 10,000

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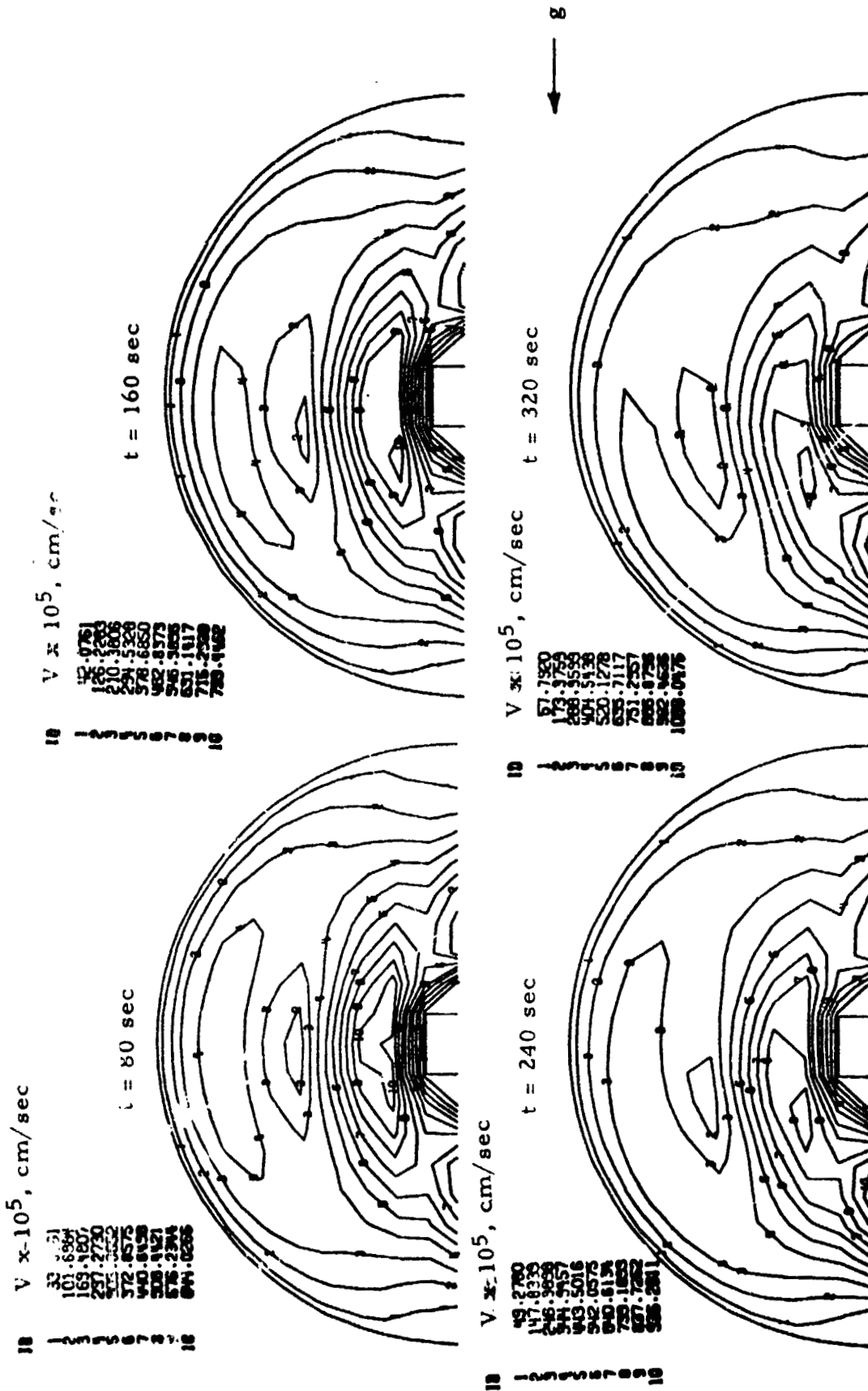Fig. 7 - Streamline Contours at Various Times for Ra = 10,000

Fig. 8 - Velocity Contours at Various Times for Ra = 10,000

CONCLUSIONS

There are a number of mechanisms other than gravity-induced convection affecting the quality of crystal growth. The results obtained in this study, therefore, must be considered in conjunction with other information in evaluating the effect of gravity on the outcome of the Lal/Kroes experiment. The results of this study indicate gravity induced convection velocities ranging from approximately 2×10^{-5} to 2×10^{-3} cm/sec for typical orbital gravity loads of 10^{-6} to 10^{-4} g_e. Although these velocities appear to be extremely small, they are comparable to the expected crystal growth rate velocities and molecular diffusion velocities.

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REFERENCE

1. Lal, R.B., and R.E. Kroes, "Experiment Requirements and Implementation Plan for Experiment MPS 770058: Solution Growth of Crystals in Zero-G," National Aeronautics and Space Administration, George C. Marshall Space Flight Center, Huntsville, Ala., August 1980.

2. Spradley, Lawrence, and M. L. Pearson, "GIM Code User's Manual for the STAR-100 Computer," NASA Contractor Report 3157, November 1979.

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