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MATHEMATICAL MODELS OF CONTINUOUS FLOW ELECTROPHORESIS.

Princeton University
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I. Fundamental Studies

(A) Synopsis

Since we are nearing the end of the contract it seems worthwhile to summarize the task, the accomplishments this far, and plans for the remainder of the contract period.

Development of high resolution continuous flow electrophoresis devices ultimately requires comprehensive understanding of the ways various phenomena and processes facilitate or hinder separation. Seemingly small individual effects may, in combination, constitute serious limitations on a particular chamber design or operating configuration, especially when particles with small mobility differences are to be separated. A comprehensive model of the actual three dimensional flow, temperature and electric fields is being developed to provide guidance in the design of electrophoresis chambers for specific tasks and means of interpreting test data on a given chamber.

Part of the process of model development includes experimental and theoretical studies of hydrodynamic stability. This is necessary to understand the origin of mixing flows observed with widegap gravitational effects, the suppression of gravity may allow other processes to become important.

To insure that the model accurately reflects the flow field and particle motion requires extensive experimental work. Much of the experimental work can be done under terrestrial conditions if the roles of gravity are appreciated and taken into account properly. Even though the resolution of a terrestrial based machine may be unsatisfactory, verification of the model will provide the support necessary for the interpretation of micro-gravity operations. Recommendations will be made for the design and operation of the ground experiments.

The research undertaken at Princeton is theoretical and computational. Supporting work at MSFC under the direction of Dr. R.S. Synder aims at establishing the experimental applicability of the theoretical work.

The principal accomplishments thus far are:

(1) A one-dimensional model of the axial and electro-osmotic flow fields was constructed and computer programs written to implement the model. The model accurately reflects the effects of temperature on viscosity, buoyancy and electro-osmotic mobility of the walls.

(2) Two-dimensional models of the temperature and flow fields were developed to evaluate edge effects.

(3) A two-dimensional model of the electro-osmotic cross-flow velocity field was constructed which includes effects of temperature on viscosity and the effect of convection on the temperature field. This model also enables one to predict the axial velocity resulting from the effect of buoyancy generated in the electro-osmotic flow.

(4) The axial development of the temperature field in the region between the electrodes was modelled to disclose a significant entrance length, heretofore unexpected.

(5) A first generation model of the separation process was constructed to predict particle separation with various chamber configurations.

(6) Several modes of hydrodynamic instability were investigated theoretically and an extreme sensitivity to small temperature gradients uncovered.

(7) Active interaction with the experimental program at MSFC was maintained. This program is a complementary effort designed to study the flow field in electrophoresis chambers and establish their operating characteristics. It has been confirmed that the aforementioned instability is the cause of meandering in wide-gap chambers at low power levels.

(8) A mathematical model which employs the so-called Hele-Shaw assumptions was developed to predict the temperature and flow fields after the meandering is established. There is good qualitative agreement with experimental results.

The following Publications have appeared:

(1) "Fluid Mechanics and Electrophoresis" in Physicochemical Hydrodynamics D. B. Spalding (Editor) Guernsey: Advance Publications, vol. 2 (1978) pp. 893-912.

(2) "Fluid Mechanics and Continuous Flow Electrophoresis" (COSPAR) Space Research, Proceedings of the XXIst COSPAR Conference (Innsbruck), vol. XIX, M.J. Rycroft (Editor) OXford: Pergamon Press (1979) pp. 583-597.

(3) "Studies of Continuous Flow Electrophoresis" AIAA paper No. 79-0032, New York: American Institute of Aeronautics and Astronautics (1979) 4 pp.

(4) "Flow and Thermal Effects in Continous Flow Electrophoresis UAH/NASA Workshop on the Fluids Experiment System (John Hendricks and Barbara Askins, Editors) Huntsville: Univ. of Alabama (1979) pp. 136-145 (with P.H. Rhodes and R.S. Snyder).

Papers in Preparation

(1) An Overview of Continuous Flow Electrophoresis [Accepted for publication in J. Physicochemical Hydrodynamics].

(2) Structure of Temperature Velocity Fields in Continuous Flow Electrophoresis.

(3) Development of the Temperature Field in a Fully Developed Laminar Flow.
[Accepted for presentation at the Philadelphia Meeting of the AIChE].

(4) Flow Structure and Temperature Fields in an Electro-osmotically Driven Flow.
[To be submitted to J. Heat Transfer, ASME].

(5) Hydrodynamic Stability of the Flow in an Electrophoresis Chamber.

(6) A Mathematical Model of the Fractionation of Cell Populations in Continuous Flow Electrophoresis.

During the remainder of the contract period we expect to:

(A) Continue our collaboration with MSFC to:

  (i) Complete the studies of meandering and stability.

  (ii) Test the separations model.

  (iii) Develop a flight experiment and improve the chamber design.

(B) Develop mathematical models of the effects of concentration polarization.

(C) Investigate the effects of axial temperature gradients on fraction.

(D) Investigate some of the effects of cell concentration, e.g. agglomeration in shear and electric fields.

(B) Current Work

(1) <u>Studies of the electro-osmotic cross-flow (Deiber)</u>

In our last progress report we described efforts to extend the results of a previous study of a weak electro-osmotic crossflow so as to include the effects of a stronger flow, including that due to leaky membranes. Since the last report we have completed an extensive revamping of the computational technique so as to include a variety of modes of electrical heating. In the earlier studies it was assumed for simplicity that the electric field was uniform throughout the chamber cross-section. Now, it is possible to make computations based on a constant current or, more realistically, the conservation of charge. The latter computation requires the simultaneous solution of the equation for the conservation of charge

$$\nabla \cdot \sigma \underline{E} = 0, \qquad (1)$$

the energy equation and the equations of motion. This has been implimented and some of the results are shown next.

Figures 1, 2, 3 and 4 depict some results from this study calculated using characteristics of the A-1 buffer and the wide-gap chamber (SPAR). Figures 1 and 2 show the situation where membrane leakage adds to the electro-osmotic flow to provide sharp temperature gradients at the right hand membrane. Figures 3 and 4 depict matters when leakage opposes electro-osmosis and indicates that a controlled leakage can diminish the sharp gradients produced by electro-osmotic convection.

Of course the temperature field depicted in Figure 2 will produce severe buoyancy effects that can alter the sturcture of the axial velocity. To probe this a computer program was devised to solve for the axial velocity due to buoyancy and pressuring forces. Figure 5 shows contours of equal axial velocities arising from buoyancy produced by the temperature field shown in Figure 2. In the absence of the asymmetric temperature field and the attendant buoyancy the (up-flow) axial velocity field (due to a pressure gradient) would be symmetric with respect to the median planes (similar to that shown on the left of Figure 5). The added buoyancy due to warm fluid adjacent to the right hand membrane causes channeling and enhances the upward flow here at the expense of flow elsewhere in the cross section.

The effects depicted here are of central importance in the design and operation of continuous flow devices in 1-g and micro-g gravity fields. If the hydrodynamic instabilities due to small temperature gradients can be suppressed by careful design then the next limits on 1-g operation will be the structure of the fully developed temperature and axial velocity fields. Buoyancy effects in upflow or downflow must, at the very least, be taken into account in deciding on locations for sample stream injection and removal. Such effects will also alter same residence times and may engender other hydrodynamic instabilities due to the sharp gradients.

Work on this aspect of the problem is complete and a manuscript has been prepared for submission to the Journal of Heat Transfer (ASME). That manuscript plus an appendix describing the computer programs in being assembled in the form of a project report to NASA.

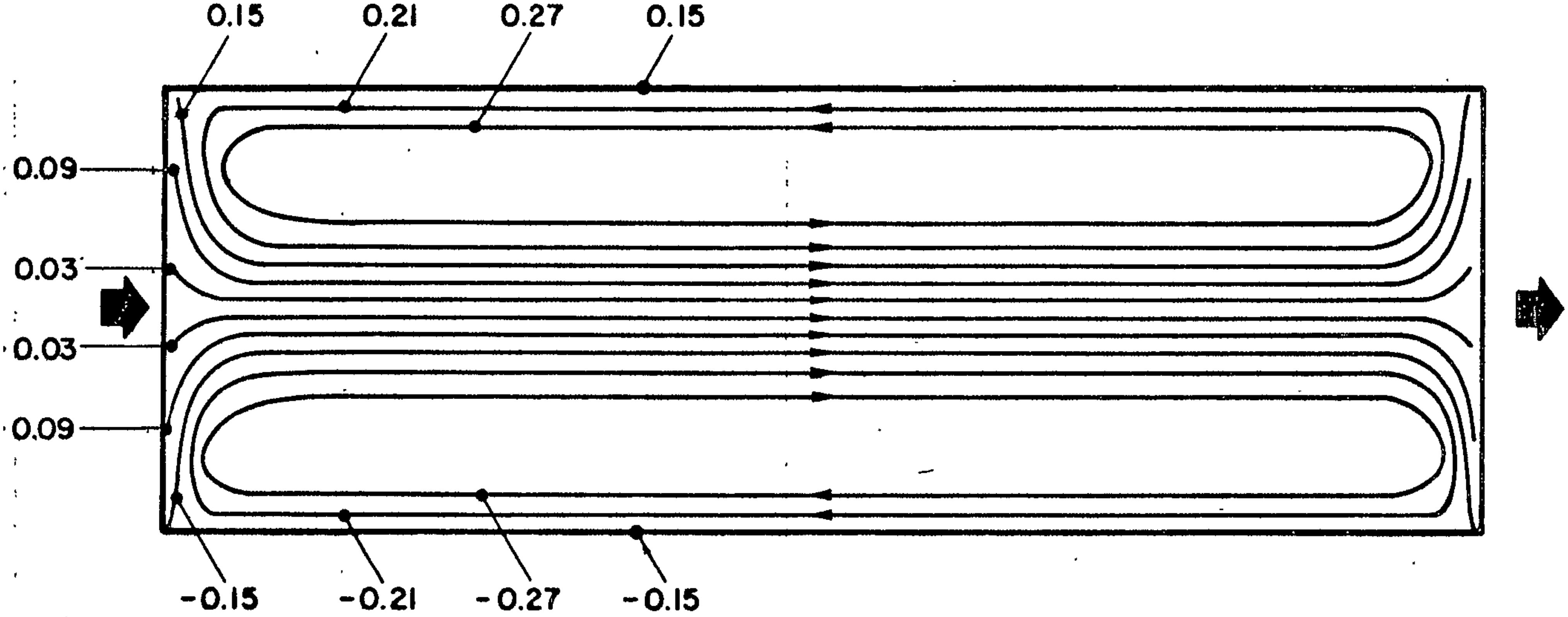
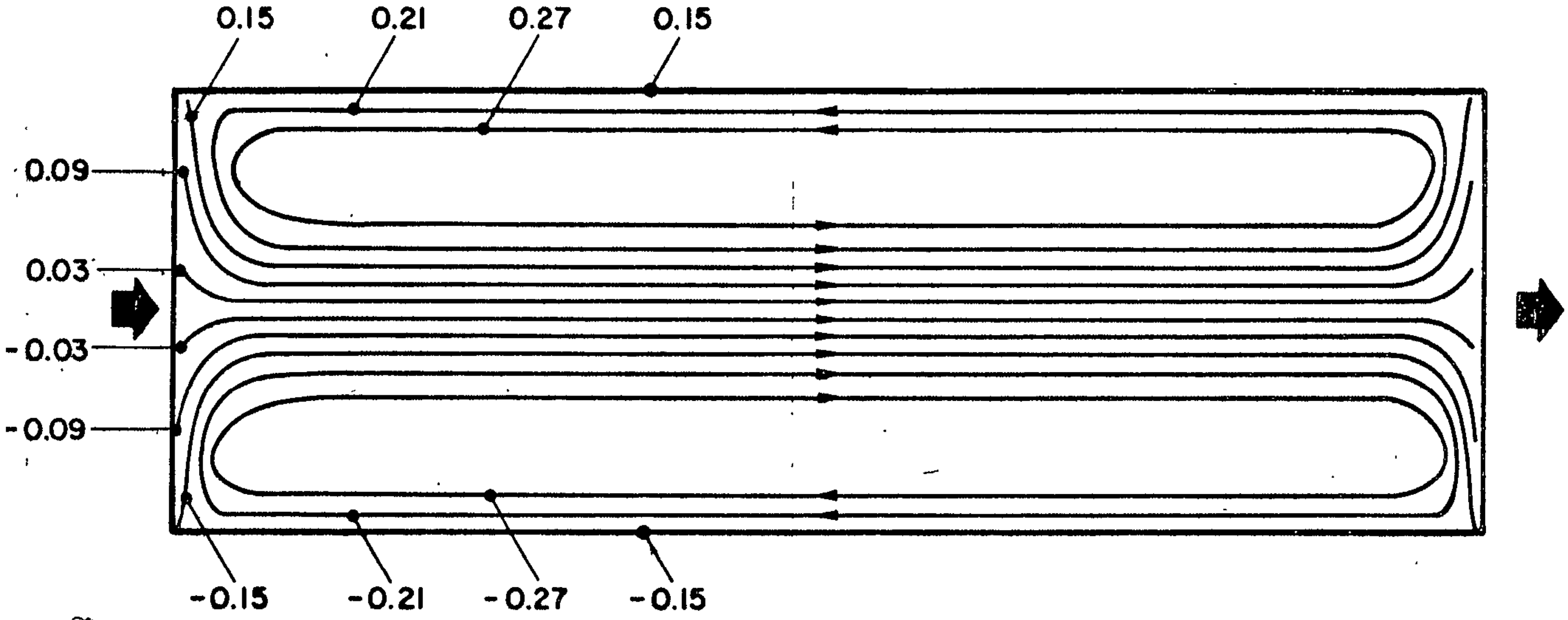


Figure 1: Flow patterns (streamlines) in a rectangular chamber due to the combined effects of leakage through the membranes and electro-osmosis. Note that the figure is not drawn to scale. The actual aspect ratio (width/depth) is 10.



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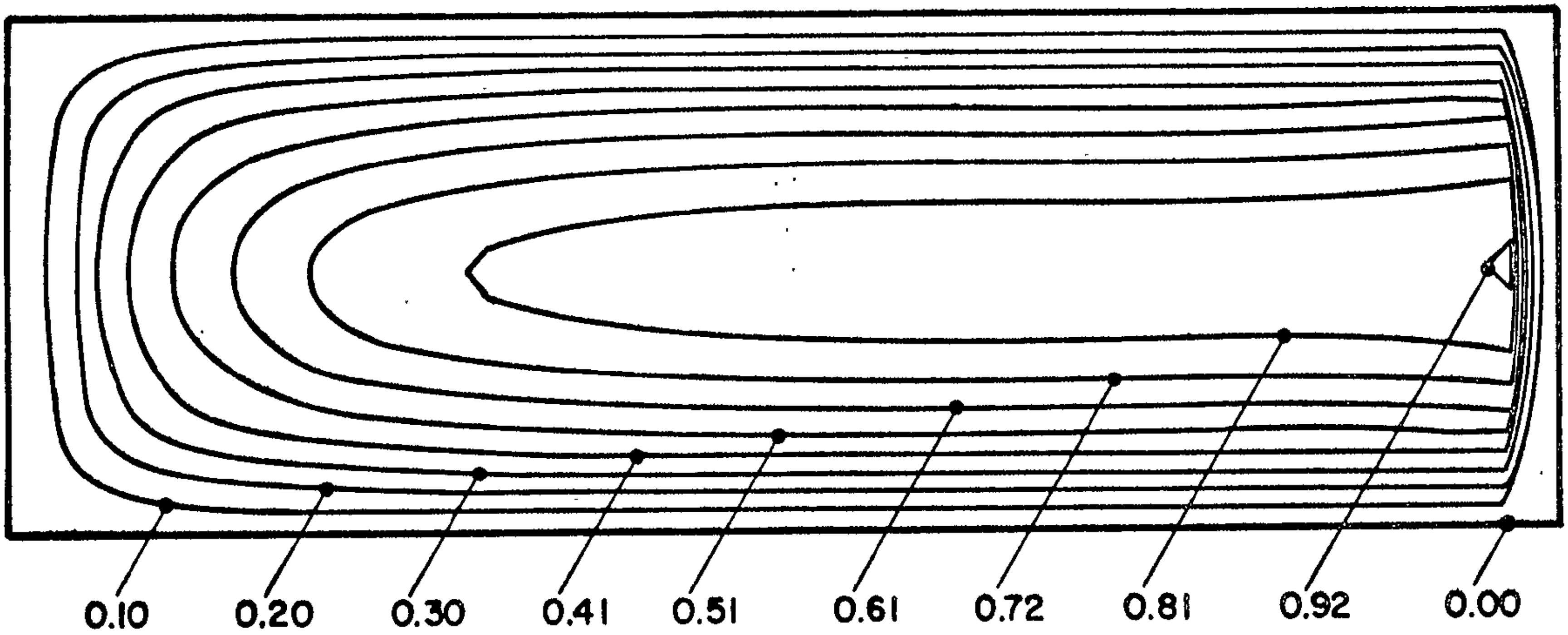


Figure 2: Isotherm pattern in the chamber flow depicted in Figure 1. Note steep temperature gradients at right.

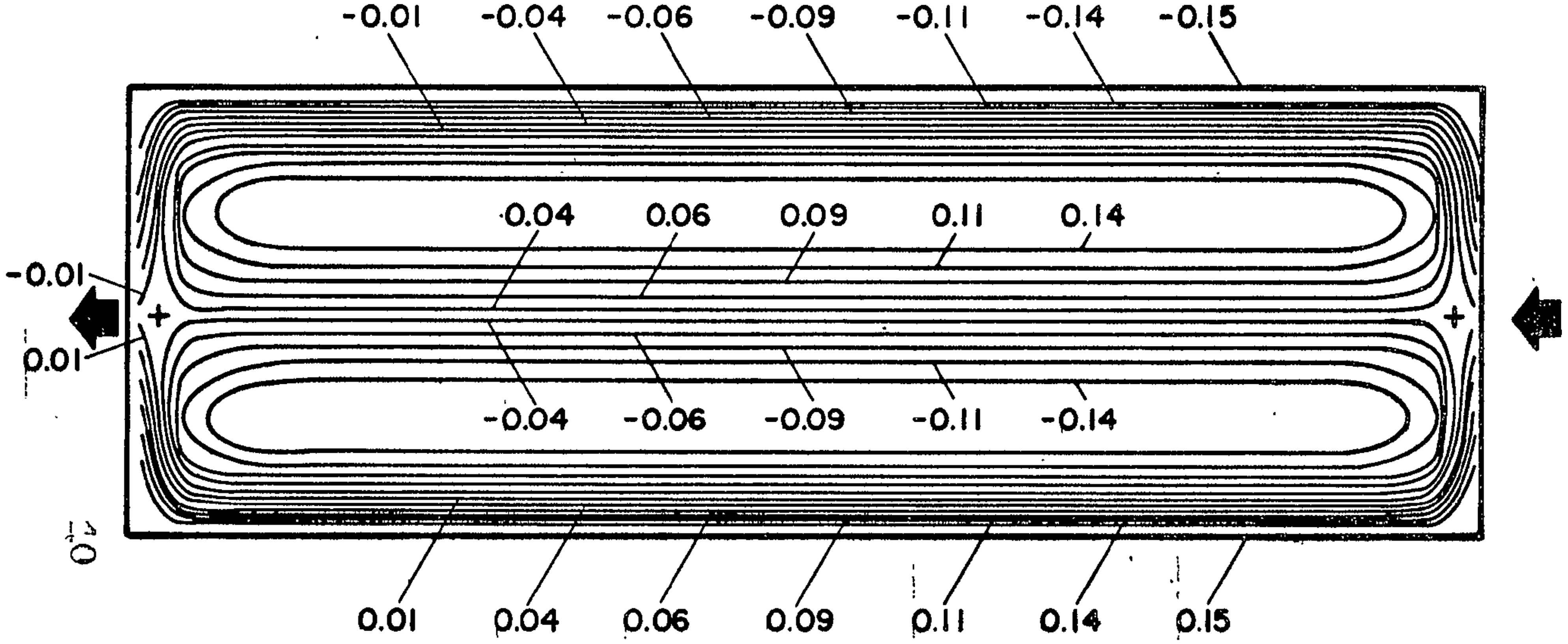


Figure 3: Flow patterns (streamlines) in a rectangular chamber due to the opposing effects of electro-osmosis and leakage through the end walls.

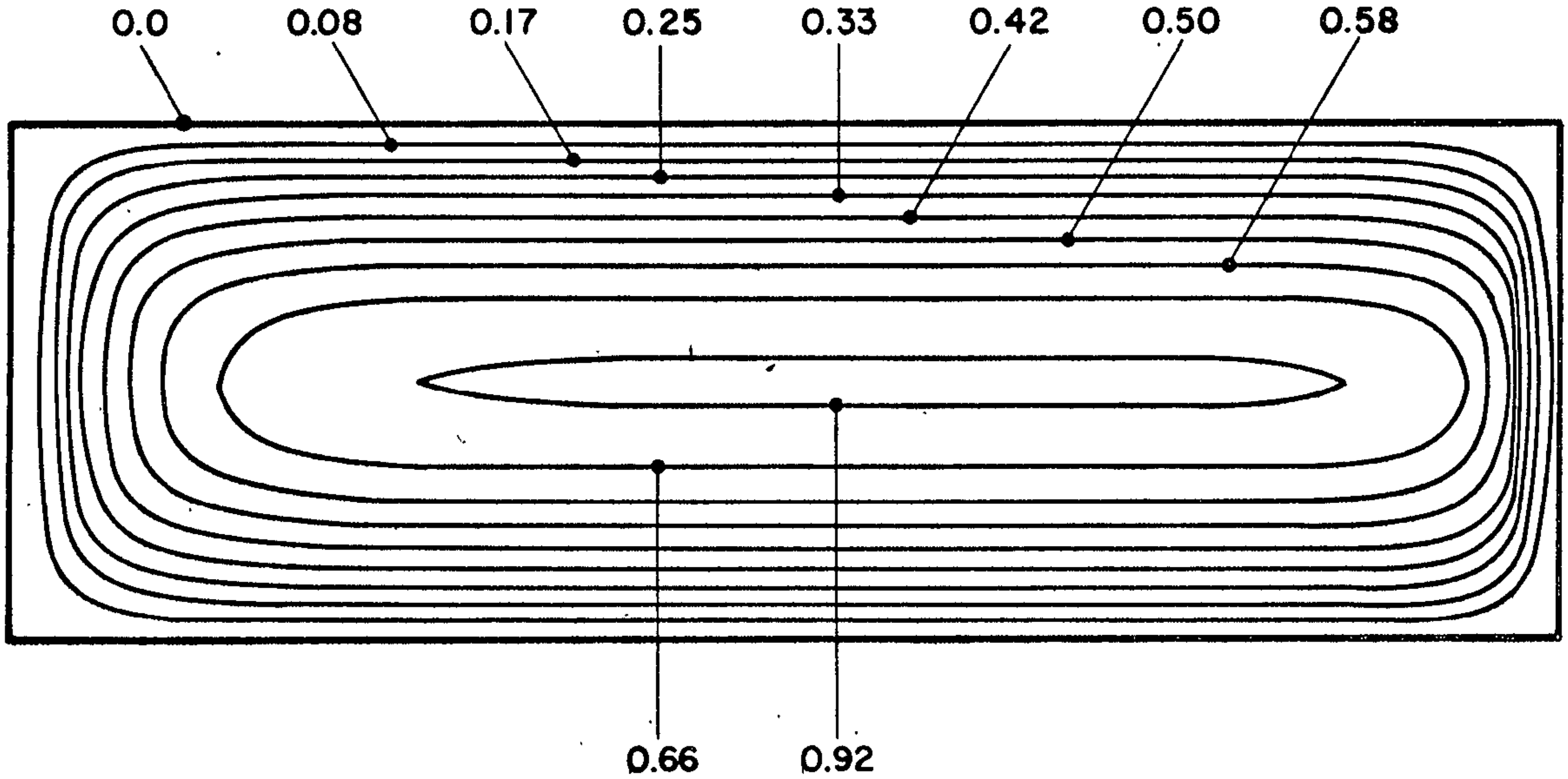


Figure 4: Isotherm pattern corresponding to the flow depicted on Figure 3.

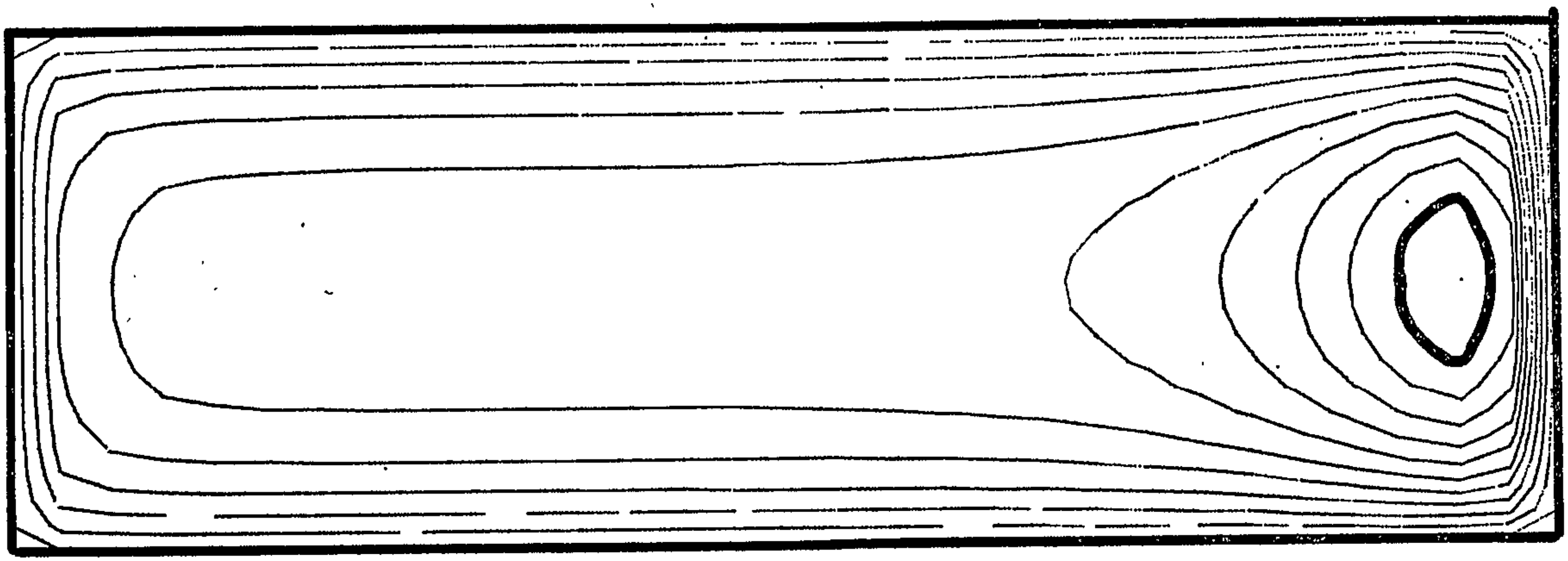


Figure 5: Contours of constant axial velocity (into the paper) due to combined effects of a pressure gradient and buoyancy for the temperature field shown on Figure 2.

(2) Flow Stability and Structure (Saville)

Recent experimental studies by P.H. Rhodes at MSFC [NASA TM-78178] disclosed, among other things, a noteworthy correspondence between the measured temperature gradients associated with flow meandering and the hydrodynamic instability noted in earlier progress reports. According to the theory, a critical axial temperature gradient exists above which the flow is unstable. For perfectly conducting walls the critical value, expressed in terms of the Rayleigh number, is

$$\frac{g\beta \frac{dT}{dz} d^4}{\nu\alpha} = 6 \qquad (2)$$

and for insulating walls the value is

$$\frac{3}{4} \frac{\pi^2}{H^2}, \quad H >> 1.$$

H is the aspect ratio (width/depth). Rhodes found strong evidence for the inception of meandering and (perhaps) recirculation at measured Rayleigh numbers in the range of 2-6. Furthermore, the structure of the flow appears to agree qualitatively with the theory.

Because the theory is constrained by several assumptions so as to yield analytical results we sought to construct an alternate model which would circumvent problems inherent in the linearized stability theory. The model developed employs the so-called Hele-Shaw assumptions, viz. variations in the y-direction (the narrow dimension or gap thickness) are averaged so that one deals with a

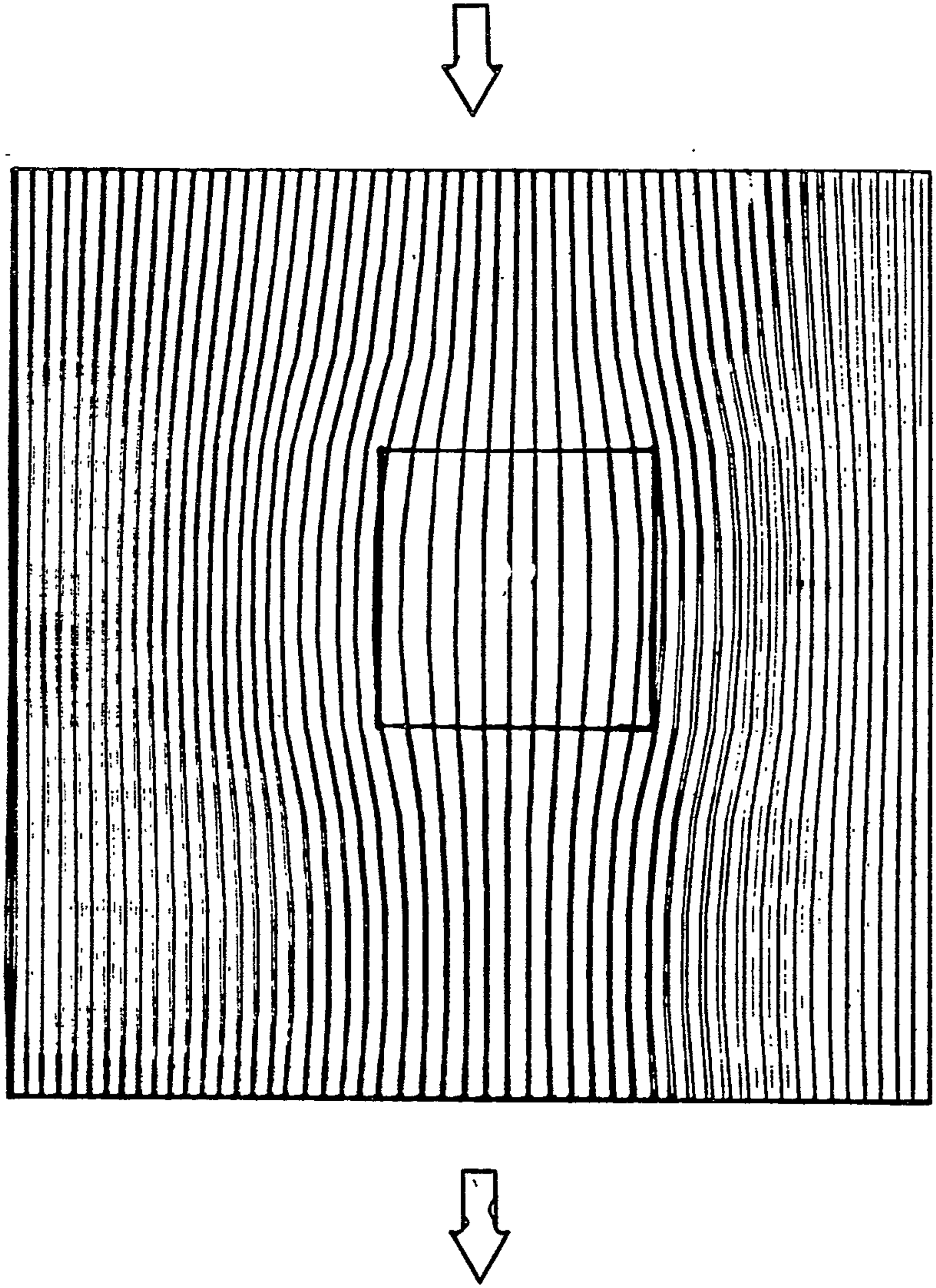
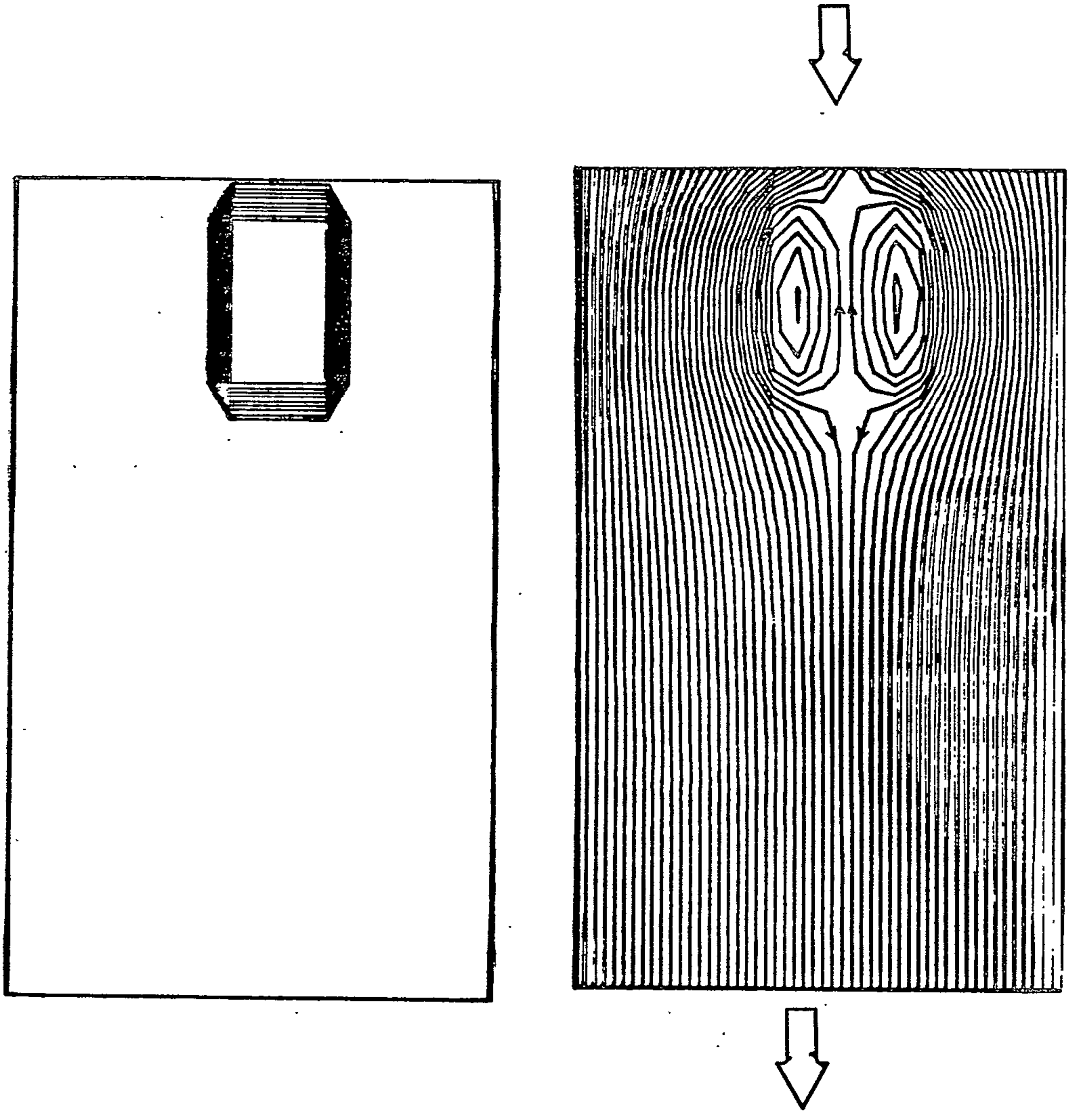


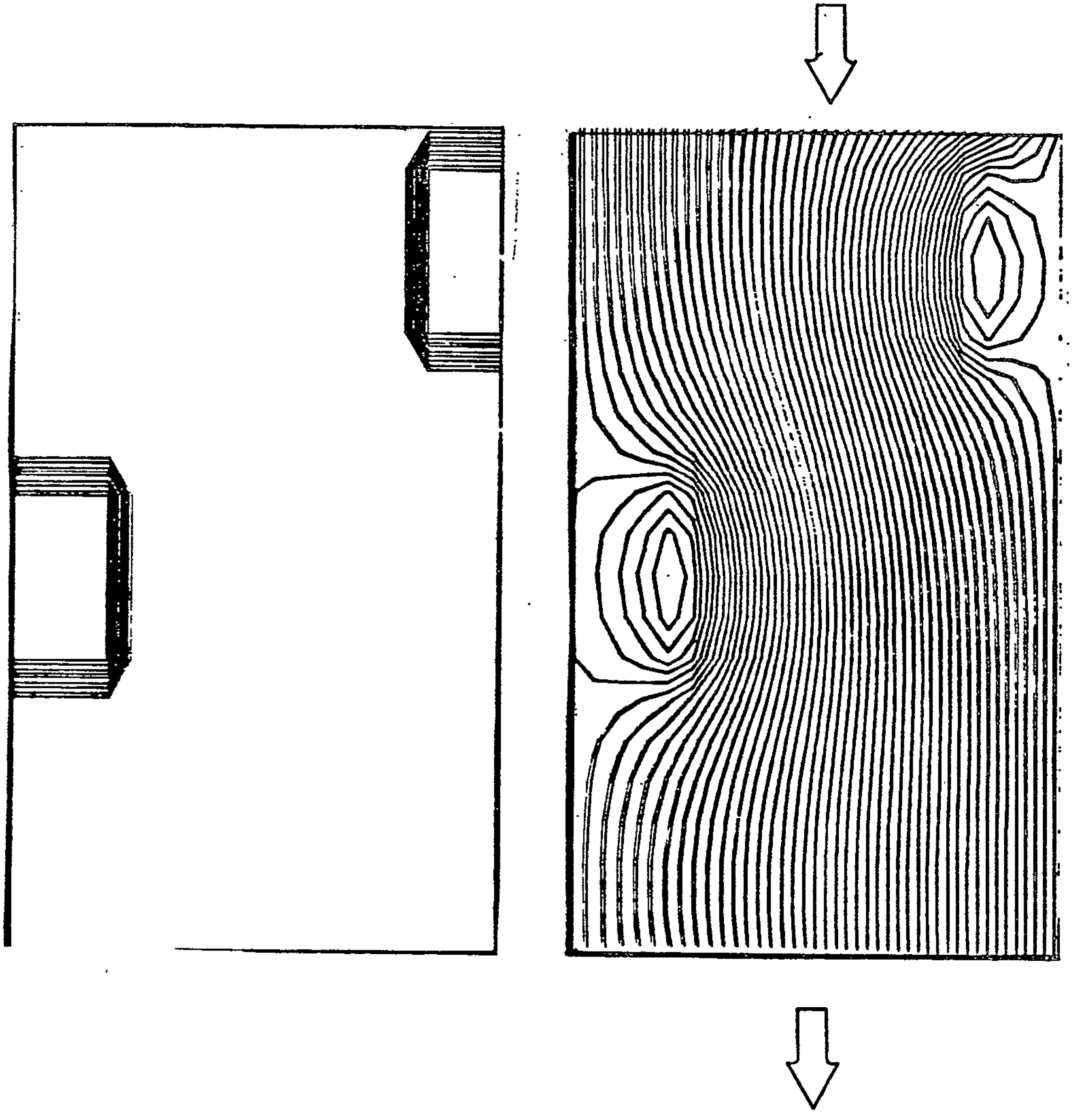
Figure 6: Streamline pattern for downflow through a square chamber with a square 'hot-spot'. Note that the slight buoyancy causes a 'repulsion' around the hot spot.



(a) Temperature Field

(b) Flow

Figure 7: (a) Assumed temperature field - maximum temperature difference between the hot spot and the rest of the chamber is 1°C.
(b) Flow field corresponding to the situation studied in Rhodes experiments. Note recirculation.



(a)

Temperature

(b)

Flow

Figure 8: (a) Assumed temperature field - two hot spots.
(b) Flow field showing two eddies.

two-dimensional problem. The equation governing the two-dimensional stream function turns out to be

$$\nabla^2\psi = -N_1\ \partial\Theta/\partial Z \qquad (3)$$

where N_1 is a dimensional group involving, among other things, buoyancy and Θ is the temperature. In the computation a known temperature field is given as input and the equation solved for the flow pattern. Figure 6 shows the streamlines for downflow at a low heating rate where $N_1 = 5$ with the square region 0.5°C hotter than the rest of the chamber. There is very little distortion. Figure 7 shows the state-of-affairs in a chamber with dimensions, flows etc. conforming to the SPAR chamber operating conditions used in Rhodes' experiments. The left hand side depicts the temperature field and shows a 'hot sport' with a maximum temperature approximately 1°C hotter than the surroundings. The streamlines on the right depict a recirculating eddy due to the effect of buoyancy in the warm region. Figure 8 shows the flow pattern which ensues when two hot spots are present, eahc with a maximum temperature 1°C higher than the surroundings.

Another interesting aspect of the Hele-Shaw approach is that by adding an equation for the conservation of energy we can examine the stability of the chamber. Such a computation involves solving an eigenvalue problem and, for the case of an insulating lateral boundary, the critical Rayleigh number is

$$\frac{3\pi^2}{4H^2}$$

which is in exact agreement with the more complicated theory for insulating boundaries. It is not possible to compare the Hele-Shaw model to the exact calculation for perfectly conducting boundaries since the requirement of isothermal front and rear faces is incompatible iwth the Hele-Shaw assumptions.

We believe the model has considerable utility both as a tool for design and for understanding the behavior of the chamber and therefore plan to pursue its development in collaboration with the experiments at MSFC.

(3) Implementation of the Separation Model (Duranceau)

Our efforts to refine and verify the mathematical model have continued with recent work devoted to comparing separations achieved in the Beckman and Hannig CPE's by J.K. McGuire of MSFC with results predicted using the model. At the same time we are preparing a documented 'users guide' so that the software can be turned over to Dr. R.S. Snyder's group at MSFC for their use. The results from the computer program can be presented in several forms, e.g.

(a) the mobility distribution in each collector stream

(b) particle distribution at the outlet plane

(c) outlines of regions containing preselected mobilities.

Some examples are given in Figures 9 and 10, which show predicted separation in the Beckman CPE. Figure 9 shows the number densities (concentrations) of particles leaving the device as a function of position. Here the input stream (injected at $Z \doteq -.55$) contained two cell populations with well separated average mobilities (cow: $\mu = 2.0$ µm/s/v/cm and turkey, $\mu = 2.9$ µm/s/v/cm) and the separation is good. Figure 10 shows the outlines of the average mobilities of the two populations-again showing good resolution.

BECKMAN CPE RESOLUTION (R-1 BUFFER)

FLOWRATE 0.43 $(cm)^3/s$
FIELDSTRENGTH 75×10^2 V/m

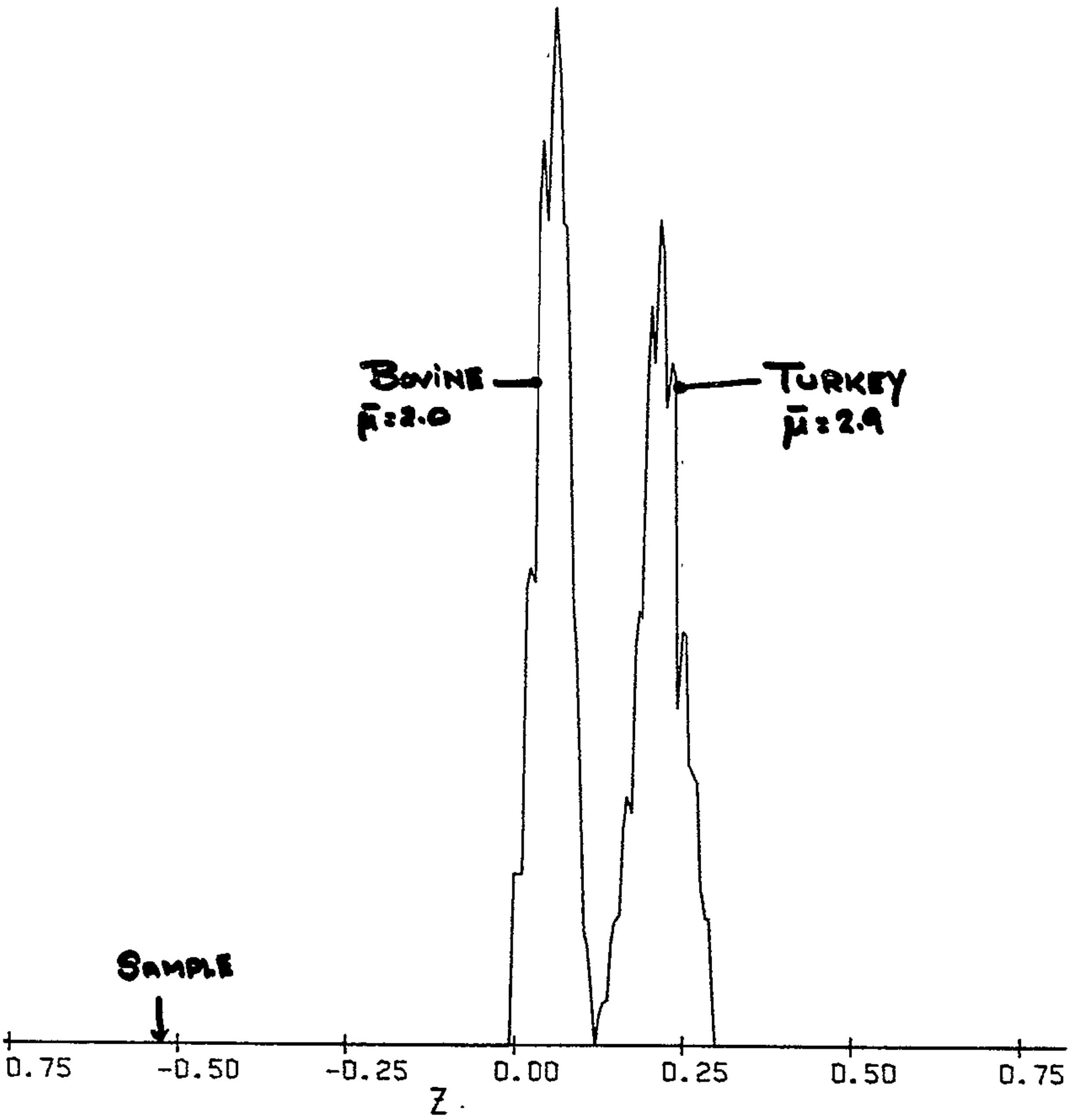


Figure 9

BECKMAN CPE RESOLUTION (R-1 BUFFER)

FLOWRATE 0.43 $(dm)^3/s$
FIELDSTRENGTH 95×10^2 v/m

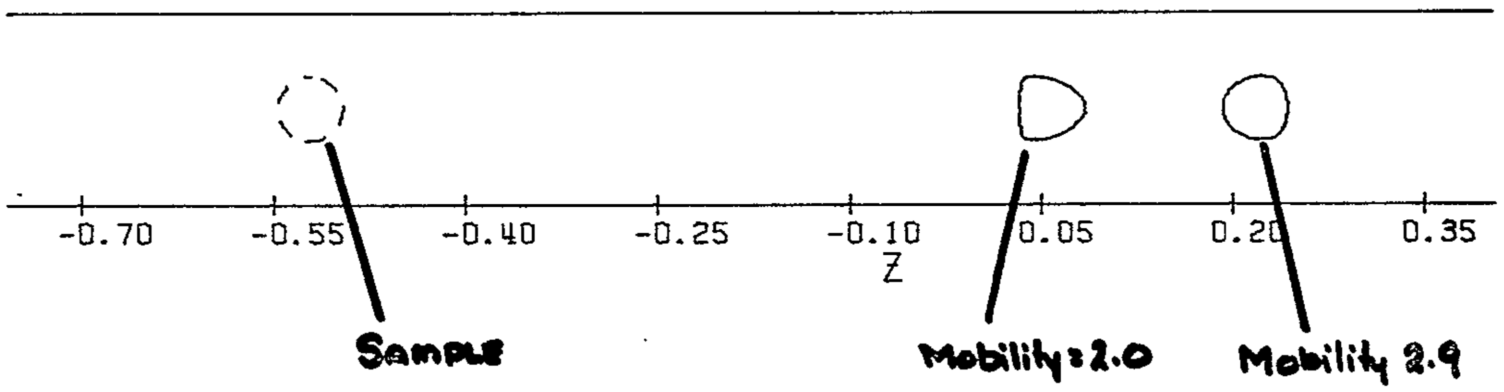


Figure 10

(4) Project Review

On October 18, 1979 a project review was held at MSFC where progress, current/status and future plans were presented and reviewed by NASA management including Dr. John Carruthers.

(5) The Fluids Experiment System Workshop

A paper on continuous flow electrophoresis coauthored with P.H. Rhodes and R.S. Snyder of MSFC was presented at the Workshop at the Universtiy of Alabama in July.

II. Plans for the next Reporting Period

During the next reporting period we plan to focus efforts on

(1) preparation of the aforementioned reports,

(2) collaborate with MSFC on studies of hydrodynamic stability;

(3) continuous testing of the separation model.