N84-24716

ANALYSIS OF ELECTROPHORESIS PERFORMANCE

Final Report
RAI-84-E-3

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ABSTRACT

Our computer code SAMPLE models electrophoresis separation in a wide range of conditions. Applications include steady three-dimensional continuous-flow electrophoresis (CFE), time-dependent gel and acetate film experiments in one or two dimensions and isoelectric focusing in one dimension. Sample results for all these are included.

The code evolves N two-dimensional radical concentration distributions in time, or distance down a CFE chamber. For each time or distance increment, there are six stages, successively obtaining the pH distribution, the corresponding degrees of ionization for each radical, the conductivity, the electric field and current distribution, and the flux components in each direction for each separate radical. The final stage is to update the radical concentrations.

The model formulation for ion motion in an electric field ignores activity effects, and is valid only for low concentrations; for larger concentrations the conductivity is therefore also invalid.

We have duplicated one-dimensional results obtained with a similar model by Bier et al.

We have successfully modeled eight experiments done with hemoglobin in a barbitol buffer on acetate film.

TABLE OF CONTENTS

Section 1

INTRODUCTION

This report is brief, and references the numbered view graphs in the Appendix.

Graphs 1 - 6 are an introduction to the presentation and to electrophoretic separation processes, and are not further described.

Section 2 and graphs 7 - 22 are a description of the model formulation, assumptions, and applications, and of the numerical methods, coding and use.

Section 3 and graphs 23 - 46 present results of analytic validations, acetate film experiment simulations, continuous flow electrophoresis simulations, and simulations of electrophoresis cases modeled by Bier et al.

This is a continuing program. Some plans for future work are presented in graph 47.

Section 2

DESCRIPTION

Graph 7 is a code summary, listing the six stages in updating N two-dimensional radical concentration distributions, and describing some available applications of the code in its present form.

Graphs 8 and 9 describe the ionization model and assumptions. All salts are fully ionized. The ionization equilibrium of each radical (or ampholyte, including proteins and cells) is a function only of pH. Four distinct ionization models are used. The coefficients are determined to fit titration measurements of the mean ionization. Graph 10 presents the mean ionization for three hemoglobin types; the root mean square difference from measurements is of order 0.1, which is excellent for magnitudes of order 20.

Graph 11 describes the calculation of the pH distribution from local charge neutrality. Newtons iteration gives very high efficiency and accuracy.

Graph 12 describes the model for ion motion and radical flux, and for the resulting changes in radical concentration. The radical flux is obtained by summing over the degrees of ionization, and has terms representing transport by the mean flow, transport proportional to the local electric field, and a diffusive flux.

The electric field distribution is calculated from charge continuity, the computed total conductivity distribution, and the computed ion diffusion current potential, as described in Graph 13.

Graph 14 discusses an improved model for ion motion, including activity effects of varying concentration. This model has not yet been finalised or implemented, but is a requirement for quantitative agreement with measurements, except at the lowest concentrations.

Applications to continuous flow electrophoresis (CFE), moving-wall CFE, and to time-dependent one and two-dimensional cases are described in Graphs 15 through 19, with the corresponding requirements for initial conditions, computational domain and boundary conditions.

Output options are listed in Graph 21.

Graph 22 show the input data, and demonstrates the code's flexibility. This data file can be modified in a few moments to make appropriate changes in the problem, the method or the output. This data is for a 3-radical computation with hemoglobin in a barbitol buffer.

Section 3

RESULTS

Analytic code validations are discussed in Graph 23. In certain simple cases and for some components of the problem, analytic solutions and simple measurements are available. The success of the code in duplicating these encourages us in applying it to much more complicated situations. Graphs 24 and 25 are contour plots showing how a weak circular hemoglobin sample preserves its shape after 40 seconds of advection in a uniform barbitol buffer with pH 8.5, with a field of 100 V/cm. This is only one of the wide range of validations we have performed.

Graphs 26 through 36 describe our successful simulations of eight hemoglobin-barbitol experiments with a circular sample in acetate film, performed in May 1983. Graph 27 is a poor reproduction of some of the original films, with the hemoglobin "fixed" by standard processing. Graphs 28 through 36 (including some plots without graph numbers) are concerned with one case, with sample 8.8% hemoglobin in a 2.5X MACDAC barbitol solution, and with a 0.75X buffer. The mean field is 12 V/cm to the left, and the computation went to 360 seconds. Graphs 31 to 3 show successive center-line concentrations of hemoglobin, barbiturate sodium; the hemoglobin spreads to the right with a low constant concentration of approximately circular shape, while the sodium and barbiturate build up on the left and are depleted on the right. Graph 34 shows the successive conductivity profiles on the center-line. The ratio of maximum to minimum increases from 2 to 50; the maximum moves to the left and a minimum forms to the right.

The following plots show the successive pH profiles, the electric field along the film (varying from 2.8 to 25 compared with a mean of 12 volts/cm), the current lines, and the transverse electric field, with peak 6 V/cm, which spreads the hemoglobin sample.

Graphs 35 through 39 are contour plots of continuous flow electrophoresis (CFE) tests, with a weak circular hemoglobin sample so that the conductivity and field remained effectively uniform. The tests include a moving wall case where the sample remains circular and CFE with electroosmosis respectively zero, negative and positive. The distortions due to nonuniform flow down the chamber and to positive electroosmosis approximately cancel in Graph 39, as predicted by theory.

Finally our successful duplication of the seven one-dimensional computation of Bier et al. is described and demonstrated in Graphs 40 through 46.

APPENDIX

Computer-generated viewgraphs numbered from 1 through 47 are presented on the following pages.

ORGANIZATION: RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: 1	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14,1984

PRESENTATION SUMMARY

- OBJECTIVES
  - DESCRIBE FORMULATION AND ASSUMPTIONS
  - DESCRIBE CODE AND CAPABILITIES
  - PRESENT VALIDATIONS AND RESULTS
  - GUIDANCE ON ELECTROCHEMISTRY AND APPLICATIONS
- OUTLINE
  - INTRODUCTION
  - DESCRIPTION
    - FORMULATION, EQUATIONS, AND ASSUMPTIONS
    - APPLICATIONS, INITIAL AND BOUNDARY CONDITIONS
    - CODING, NUMERICAL METHODS, AND USE
  - RESULTS
    - ANALYTIC VALIDATIONS
    - ACETATE FILM EXPERIMENTS
    - CONTINUOUS FLOW ELECTROPHORESIS
    - BIER GROUP CASES
  - PLANS
    - IMPROVE OUTPUT OPTIONS (MOVIES)
    - IMPROVE FORMULATION
    - INTERACTION WITH EXPERIMENTS
    - ADD DYNAMICS IF APPROPRIATE

14-FEB-84 07:29

ORGANIZATION: RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: INTRODUCTION- 2	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 10, 1984

PROTEIN SEPARATION BY ELECTROPHORETIC MOBILITY AT VARYING pH

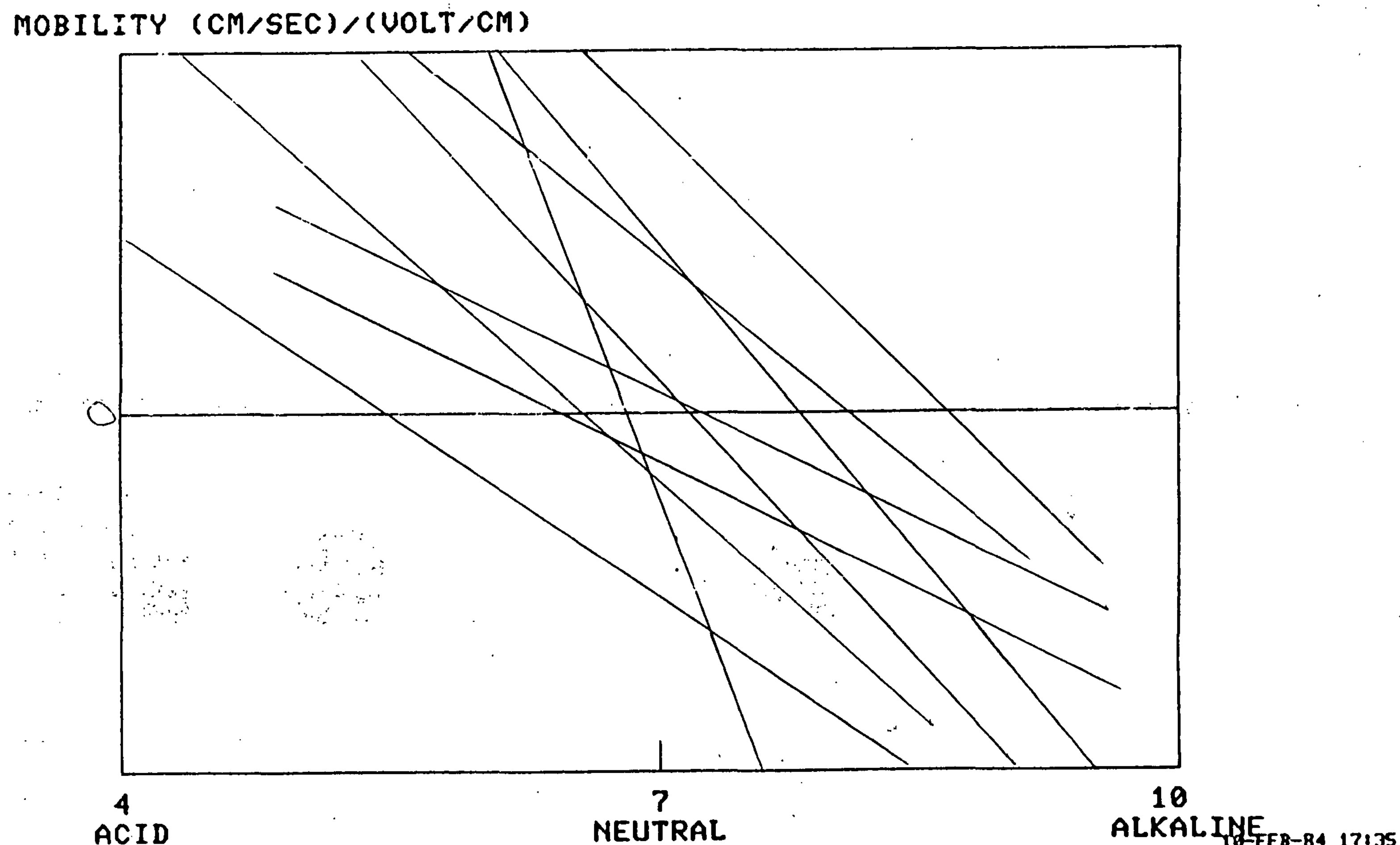

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CHART NO.: INTRODUCTION- 3	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 10, 1984

CONTINUOUS FLOW ELECTROPHORESIS (CFE)

CROSS SECTIONS

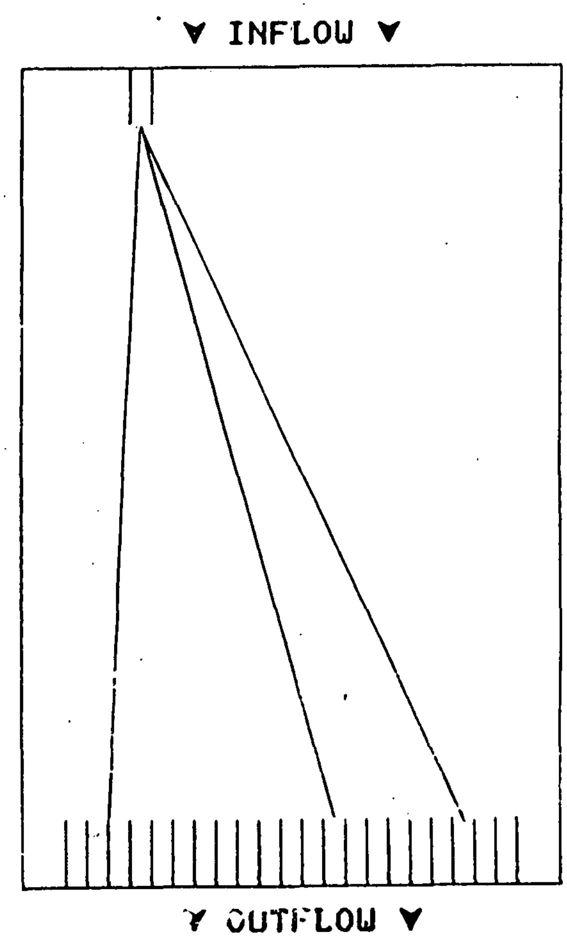
INJECTION PORT

0

➤ ELECTRIC FIELD ➤

COLLECTION PORTS

0000000000000000000000



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ORGANIZATION: RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: INTRODUCTION- 4	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14, 1984

PROBLEMS WITH CFE

- WALL FRICTION AND WALL ELECTRO-OSMOSIS
  - DISTORTS CROSS SECTIONS TO CRESCENTS
  - RESULTING RESTRICTIONS ON RADIUS
  - BUT THIS RESTRICTS THROUGHPUT
  - ALLEVIATED BY PLANNED MOVING-WALL APPARATUS
- NON-UNIFORM ELECTRIC FIELD
  - DISTORTS CROSS SECTION AND OFTEN INCREASES IT
  - AGGRAVATES DISTORTION BY WALL EFFECTS
  - CAUSED BY NON-UNIFORM CONDUCTIVITY DUE TO SAMPLE
  - ALLEVIATED BY LOW CONCENTRATIONS
  - BUT THIS RESTRICTS THROUGHPUT
- NON-UNIFORM FLOW ALONG COLUMN
  - CAUSED BY CHAMBER SHAPE AND DESIGN AND ENTRY FLOW
  - CAUSED BY CONVECTION, DUE TO OHMIC HEATING AND GRAVITY
  - ALLEVIATED BY SMALL CHAMBER DIMENSIONS
  - BUT THIS RESTRICTS THROUGHPUT
- MYSTERY PROBLEMS
  - A/C FIELD TURNS SAMPLE COLUMN TO A RIBBON
  - CERTAIN SAMPLES APPEAR TO BREAK DOWN

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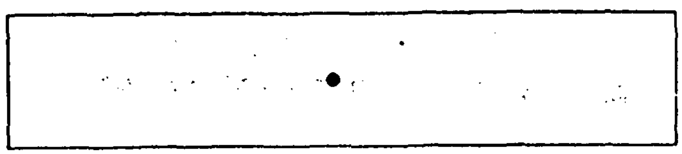
CHART NO.: INTRODUCTION- 5		DATE: FEBRUARY 10,1984

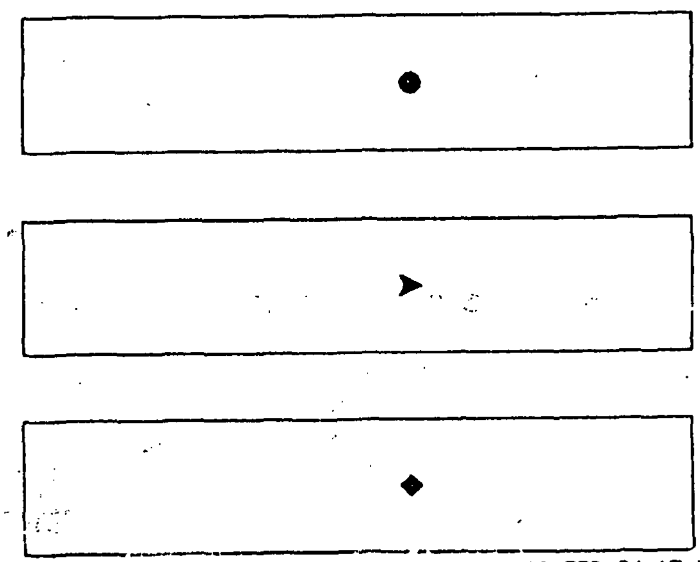
TWO-DIMENSIONAL ELECTROPHORESIS EXPERIMENTS WITH ACETATE FILM

THIS SYSTEM WAS DESIGNED FOR ONE-DIMENSIONAL ELECTROPHORESIS, WITH LINEAR SAMPLES. WE HAVE USED IT FOR CFE STUDIES, WITH CIRCULAR SAMPLES.

INITIAL SAMPLE



FINAL SAMPLES (TYPICAL)



10-FEB-84 17:36

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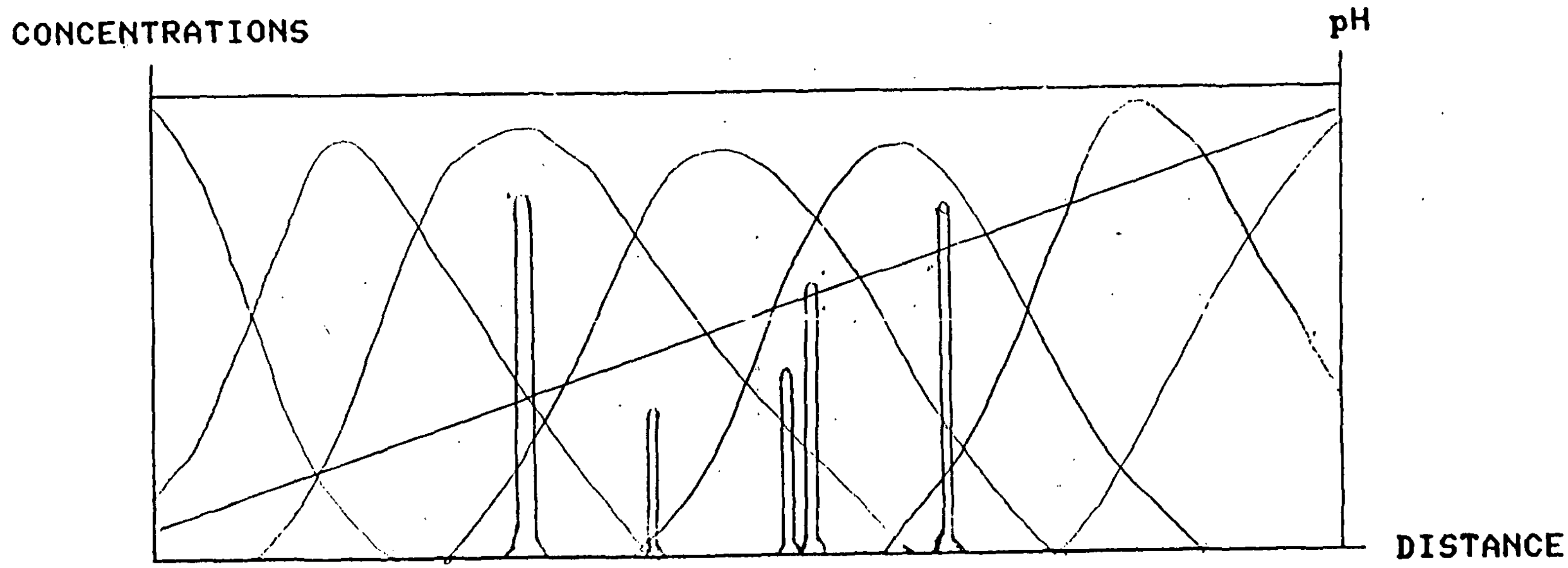
CHART NO.: INTRODUCTION- 6	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 10,1984

ISOELECTRIC FOCUSING

THIS IS A DIAGNOSTIC METHOD OF WIDE BIOCHEMICAL APPLICATION.

ELECTROLYSIS OF AN AMPHOLYTE MIXTURE IN A GEL BETWEEN IMPERMEABLE ELECTRODES ESTABLISHES A STEADY pH GRADIENT. AMPHOLYTES, INCLUDING ANY PROTEINS, ARE FOCUSED AT THE pH VALUE AT WHICH THEIR MEAN IONIZATION IS ZERO.
SMALL AMPHOLYTE MOLECULES HAVE LARGER DIFFUSIVITIES, AND ARE DISTRIBUTED OVER A RANGE SURROUNDING THEIR EQUILIBRIUM POINT, WHILE LARGE PROTEIN MOLECULES ARE SHARPLY FOCUSED.



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CODE SUMMARY

N TWO-DIMENSIONAL RADICAL CONCENTRATION DISTRIBUTIONS ARE EVOLVED IN TIME, OR IN DISTANCE DOWN A CFE CHAMBER.

THE RADICALS MAY BE SODIUM, SULFATE, ACETATE, AMMONIUM, BARBITURATE HISTIDINE, OR HEMOGLOBIN, FOR EXAMPLES.

THERE ARE SIX STAGES FOR EACH INCREMENT OF TIME OR DISTANCE:
- GET THE pH DISTRIBUTION FROM THE LOCAL IONIZATION EQUILIBRIUM;
- GET THE CORRESPONDING MEAN AND MEAN SQUARE DEGREES OF IONIZATION;
- GET THE CORRESPONDING CONDUCTIVITY DISTRIBUTION;
- SOLVE FOR THE ELECTRIC FIELD AND CURRENT DISTRIBUTIONS;
- GET THE FLUXES IN EACH DIRECTION FOR EACH SEPARATE RADICAL;
- UPDATE THE RADICAL CONCENTRATION DISTRIBUTIONS BY APPLYING AN IMPLICIT METHOD TO THE FLUX DIVERGENCES.

ONE-DIMENSIONAL CASES CAN BE DONE AS AN OPTION.

APPLICATIONS INCLUDE:
- STEADY THREE-DIMENSIONAL CFE SOLUTIONS;
- STEADY THREE-DIMENSIONAL MOVING-WALL CFE SOLUTIONS;
- STEADY TWO-DIMENSIONAL MOVING-WALL CFE SOLUTIONS;
- TIME-DEPENDENT TWO-DIMENSIONAL ACETATE FILM EXPERIMENTS;
- TIME-DEPENDENT ONE-DIMENSIONAL ACETATE FILM EXPERIMENTS;
- TIME-DEPENDENT ONE-DIMENSIONAL ISOTACHOPHORESIS;
- TIME-DEPENDENT ONE-DIMENSIONAL MOVING BOUNDARY ELECTROPHORESIS;
- STEADY OR TIME-DEPENDENT ONE-DIMENSIONAL ISOELECTRIC FOCUSING.

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CHART NO.: DESCRIPTION— 8	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14, 1984

IONIZATION MODEL

ALL SALTS ARE FULLY IONIZED.

RADICALS IN AQUEOUS SOLUTION HAVE A DEGREE OF IONIZATION DEPENDING ONLY ON THE HYDROGEN ION CONCENTRATION:

$$H = 10^{-pH}.$$

THERE ARE AT PRESENT FOUR IONIZATION MODELS AVAILABLE:

1. STRONG ACIDS AND BASES ARE ASSUMED TO BE FULLY IONIZED, TO AN IMPOSED DEGREE.

2. WEAK ACIDS, WEAK BASES, AND AMPHOLYTES HAVE CONCENTRATIONS OF EACH DEGREE OF IONIZATION IN THE RATIOS

$$\begin{aligned} & \cdots\cdots : A^{--} : A^{-} : A : A^{+} : A^{++} : \cdots\cdots \\ = & \cdots\cdots : \frac{K_1K_2}{H^2} : \frac{K_1}{H} : 1 : \frac{H}{C_1} : \frac{H^2}{C_1C_2} : \cdots\cdots \\ = & \cdots\cdots : a_{-2}H^{-2} : a_{-1}H^{-1} : 1 : a_1H^1 : a_2H^2 : \cdots\cdots \end{aligned}$$

WHERE THE CONSTANTS C AND K ARE GIVEN, FROM MEASUREMENTS. FOR A MONOVALENT WEAK ACID THERE IS ONLY ONE CONSTANT, K_1.

THEN $\quad m = \sum J a_J H^J / \sum a_J H^J , \quad M = \sum J^2 a_J H^J / \sum a_J H^J .$

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IONIZATION MODEL (continued)

3. WEAK ACIDS, WEAK BASES, AND AMPHOLYTES WITH EACH IONIZATION INDEPENDENT OF THE OTHERS HAVE

$$m = \sum H/(C_J+H) \; - \; \sum K_J/(K_J+H)$$

4. COMPLEX PROTEINS CAN IONIZE UP 30 OR MORE TIMES. WE THEREFORE USE ANALYTIC FORMULATIONS FOR m AND M :

$$m = a_0 - \sum_1^N a_i \ln\left[\frac{H + t_i}{H + b_i}\right] / \ln(t_i/b_i) \quad ,$$

WITH $N = 1$, m DECREASES SMOOTHLY FROM a_0 TO $a_0 - a_1$ AS pH INCREASES FROM $-\log(t_1)$ TO $-\log(b_1)$.

IN PRACTICE WE USE $N = 4$, AND GET THE 13 COEFFICIENTS BY A LEAST SQUARES FIT TO MEASURED MEAN IONIZATION DATA.

WITH 19 DATA POINTS FOR ONE HEMOGLOBIN TYPE, THIS GIVES A ROOT MEAN SQUARE ERROR OF LESS THAN 0.10.

THE MEAN SQUARE DEGREE OF IONIZATION M, FOR ALL FOUR MODELS, IS

$$M = m^2 + H\,dm/dH \quad .$$

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CHART NO.: DESCRIPTION- 10	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 10, 1984

IONIZATION MODEL (continued)
MEAN IONIZATION AT VARYING pH

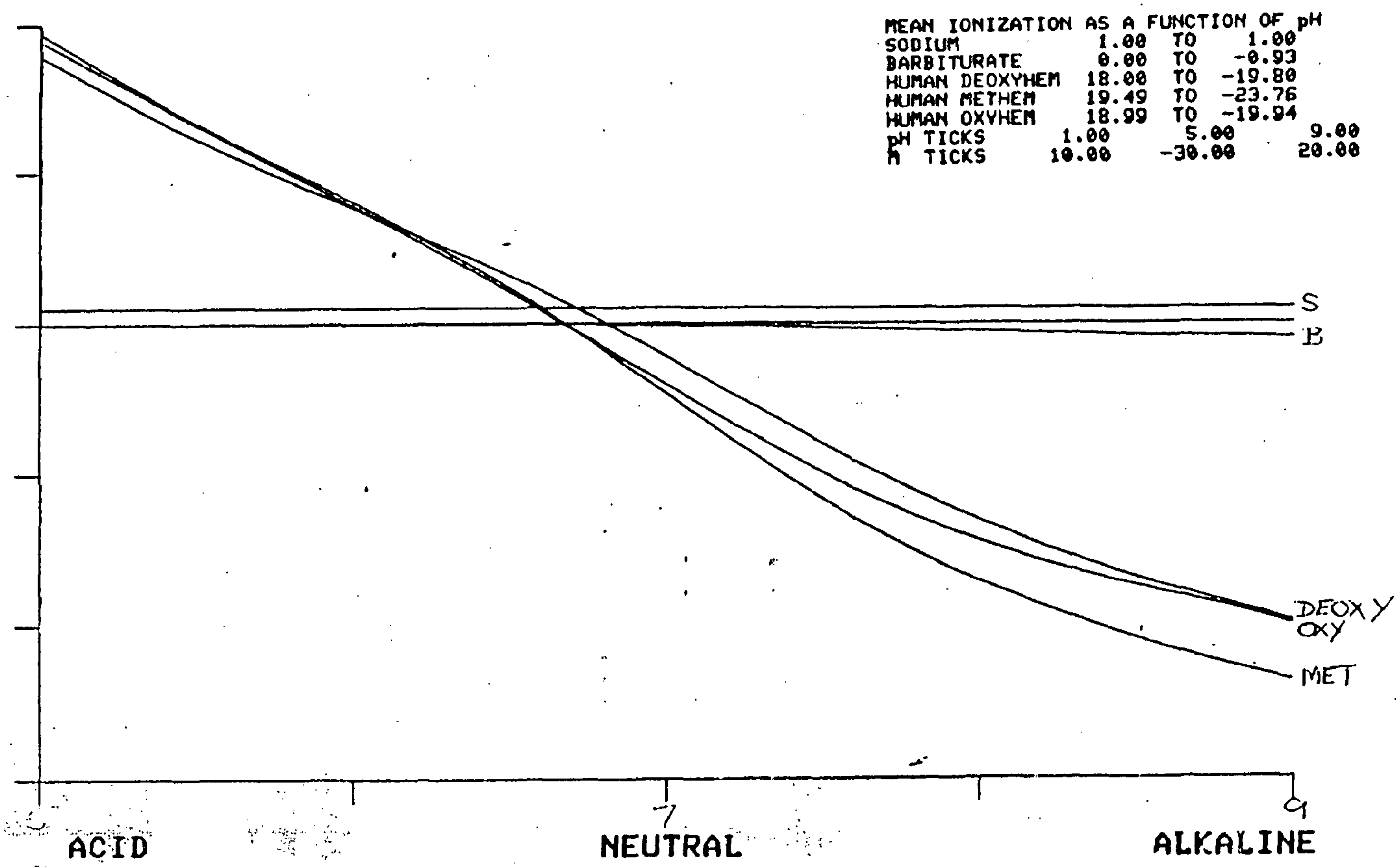

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CHART NO.: DESCRIPTION– 11	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14,1984

pH DISTRIBUTION FROM CHARGE NEUTRALITY

THE CHARGE DENSITY IS NEGLIGIBLE COMPARED WITH ITS COMPONENTS. HENCE

$$\sum_{1}^{N} c_i m_i(H) + H - K_w/H = 0$$

WHERE K_w IS THE IONIZATION CONSTANT FOR WATER, 10^{-14}.

THIS EQUATION DETERMINES H, AS A FUNCTION OF THE LOCAL CONCENTRATIONS c_i.

THE SOLUTION IS UNIQUE, SINCE EVERY TERM IS MONOTONIC.

THE CODE USES NEWTON'S ITERATION, WHICH REQUIRES dm/dH.

ONE ITERATION IS ALWAYS SUFFICIENT EXCEPT AT THE FIRST STEP.

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ION MOTION AND FLUX AND THE SPECIES CONCENTRATION

ASSUME THAT EACH ION MOVES INDEPENDENTLY THROUGH THE FLUID WITH VELOCITY

$$\underline{E} n U ,$$

WHERE n IS THE DEGREE OF IONIZATION,
U IS THE MOBILITY PER UNIT IONIZATION (ASSUMED CONSTANT),
$\underline{E}$ IS THE ELECTRIC FIELD VECTOR.

FROM CONSERVATION, THE CONCENTRATIONS (mmole/cc) OBEY

$$\dot{c}_i = - \nabla . \underline{F}_i \quad ,$$

WHERE THE VECTOR FLUX OF RADICAL i IS OBTAINED BY SUMMING OVER THE DEGREES OF IONIZATION AS

$$\underline{F}_i = c_i (\underline{u}_f + \underline{E} m_i U_i) - D_i \nabla c_i \quad .$$

HERE $\underline{u}_f$ IS THE FLUID VELOCITY, VARIES WITH THE APPLICATION, AND IS AT PRESENT ZERO EXCEPT FOR CFE,
D_i IS THE EINSTEIN DIFFUSIVITY

$$U_i RT/F \quad ,$$

R IS THE GAS CONSTANT (joules/deg/mmole) ,
F IS THE FARAD (cbs/mmole) .

ELECTRIC FIELD AND CURRENT DISTRIBUTIONS

WE IMPOSE EITHER THE MEAN ELECTRIC FIELD OR THE MEAN CURRENT DENSITY.

THE ELECTRIC FIELD HAS ZERO CURL, AND IS MINUS THE GRADIENT OF THE POTENTIAL. THE CURRENT VECTOR HAS ZERO DIVERGENCE AND IS THE CURL OF THE CURRENT FUNCTION.

THESE TWO EQUATIONS LEAD TO POISSON-LIKE EQUATIONS FOR EITHER THE POTENTIAL OR THE CURRENT FUNCTION.

EITHER EQUATION IS SOLVED USING FINITE DIFFERENCES AND AN ALTERNATING DIRECTION IMPLICIT (ADI) ITERATIVE METHOD.

THE CURRENT VECTOR IS OBTAINED BY SUMMING OVER IONS AND SPECIES AS

$$\underline{J} = \sigma \underline{E} + \nabla P ,$$

WHERE THE CONDUCTIVITY AND ION DIFFUSION CURRENT POTENTIAL ARE

$$\sigma = F (c_i M_i U_i + H U_H + K_w U_{OH}/H) .$$
$$P = RT(c_i m_i U_i + H U_H - K_w U_{OH}/H) .$$

THERE IS NO CURRENT CONTRIBUTION FROM THE FLUID VELOCITY, BECAUSE THE CHARGE DENSITY IS ZERO.

P IS ZERO IF THE MOBILITIES ARE ALL EQUAL, FROM CHARGE NEUTRALITY.

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CHART NO.: DESCRIPTION- 14	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14,1984

DEBYE-HUCKEL-ONSAGER MODEL FOR RETARDED ION MOTION

EACH ION HAS AN ATMOSPHERE OF MEAN CHARGE WITH THE OPPOSITE SIGN. FROM BOLTZMAN'S EQUATIONS, THE RADIUS VARIES WITH THE SQUARE ROOT OF THE CONCENTRATION.

THE ION MOTION IS RETARDED BY TWO EFFECTS:

FIRST, THE FLUID AT THE ION IS MOVING IN THE OPPOSITE DIRECTION BECAUSE OF THE FORCE ON THE CHARGED CLOUD.

SECONDLY, THE CLOUD ITSELF IS DISPLACED BY THE FIELD. THIS REDUCES THE FIELD AT THE ION.

THESE EFFECTS CHANGE THE ION VELOCITY THROUGH THE FLUID TO

$$(1-B)n\underline{E}U ,$$

WHERE 1-B IS THE ACTIVITY.

APPROXIMATE ANALYTIC FORMULATIONS ARE BEING DEVELOPED FOR B, OF ORDER THE SQUARE ROOT OF THE CONCENTRATIONS. THEY WILL BE TESTED AGAINST MEASUREMENTS.

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CHART NO.: DESCRIPTION- 15	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14,1984

APPLICATION TO CONTINUOUS FLOW ELECTROPHORESIS

TAKE THE x AXIS ALONG THE CHAMBER.
TAKE THE y AXIS ACROSS THE CHAMBER.
TAKE THE z AXIS IN THE FIELD DIRECTION.

THEN

$$\underline{u}_f = \left(3U(1-y^2/Y^2)/2 \ , \ 0 \ , \ E_z U_w (3y^2/Y^2 - 1)/2 \right)$$

WHERE U IS THE MEAN FLOW
$2Y$ IS THE CHAMBER THICKNESS,
y IS MEASURED FROM THE MID-PLANE,
$E_z U_w$ IS THE CONSTANT ELECTRO-OSMOSIS WALL SLIP VELOCITY.

THE RADICAL CONCENTRATION EQUATION BECOMES

$$u(y)\dot{c}_i = - \nabla . \underline{F}_i \ ,$$

WHERE THE VECTOR FLUX OF RADICAL i IS NOW ONLY TWO-DIMENSIONAL,
THE NEW TIME VARIABLE IS THE RESIDENCE TIME $t = x / U$,
AND

$$u = 3(1 - y^2/Y^2)/2 \ .$$

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OTHER APPLICATIONS

- MOVING-WALL CFE
  - WALL SPEED $E_z U_w$ IS STILL IMPOSED; IT MAY BE ZERO.
  - $u = 1 + (U_b - 1)(3y^2/Y^2 - 1)/2$
  - U_b IS THE RATIO OF THE WALL SPEED TO THE MEAN

- TIME-DEPENDENT ONE- AND TWO-DIMENSIONAL CASES
  - THE FLUID FLOW IS ZERO. USE $U_b = 1$ TO TIME STEP.
  - THE BOUNDARY AND INITIAL CONDITIONS DIFFERENTIATE THE CASES

INITIAL CONDITIONS

TWO SETS OF INITIAL CONCENTRATIONS ARE SPECIFIED, FOR THE BUFFER AND SAMPLE RESPECTIVELY.

THE SAMPLE IS CIRCULAR, CENTERED AT $(y_s, 0)$, WITH RADIUS r_s .
THE CONCENTRATION DISCONTINUITY IS SMOOTHED USING p_s .

THESE CONDITIONS ARE SUFFICIENTLY GENERAL FOR ALL APPLICATIONS SO FAR.

FOR ISOELECTRIC FOCUSING THE FINAL STEADY STATE IS INDEPENDENT OF THE INITIAL DISTRIBUTION

FOR ISOTACHOPHORESIS AND MOVING-BOUNDARY ELECTROPHORESIS THERE IS NO SAMPLE, THERE ARE TWO BUFFERS WITH A PLANE INTERFACE. THE CODE USES THE z-DOMAIN $[0\ ,\ 2r_s]$. THE LEFT BUFFER IS THE SAMPLE.

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CHART NO.: DESCRIPTION- 18	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14,1984

COMPUTATIONAL DOMAIN

FOR THE ONE-DIMENSIONAL CASES, THE y-DOMAIN IS ARTIFICIAL.
WE MAKE Y VERY SMALL, AND USE ONE INTERIOR MESH POINT.

EXCEPT FOR ISOELECTRIC FOCUSING, THE z-DOMAIN IS EFFECTIVELY INFINITE.

THE BOUNDARIES OF OUR COMPUTATIONAL DOMAIN CAN BE FIXED AT THEIR IMPOSED INITIAL VALUES, OR THEY CAN MOVE WITH IMPOSED CONSTANT VELOCITIES.
THIS GIVES OPTIMAL RESOLUTION OF THE EVOLVING SAMPLE SHAPE.

THIS IS ILLUSTRATED IN THE NEXT VIEWGRAPH.

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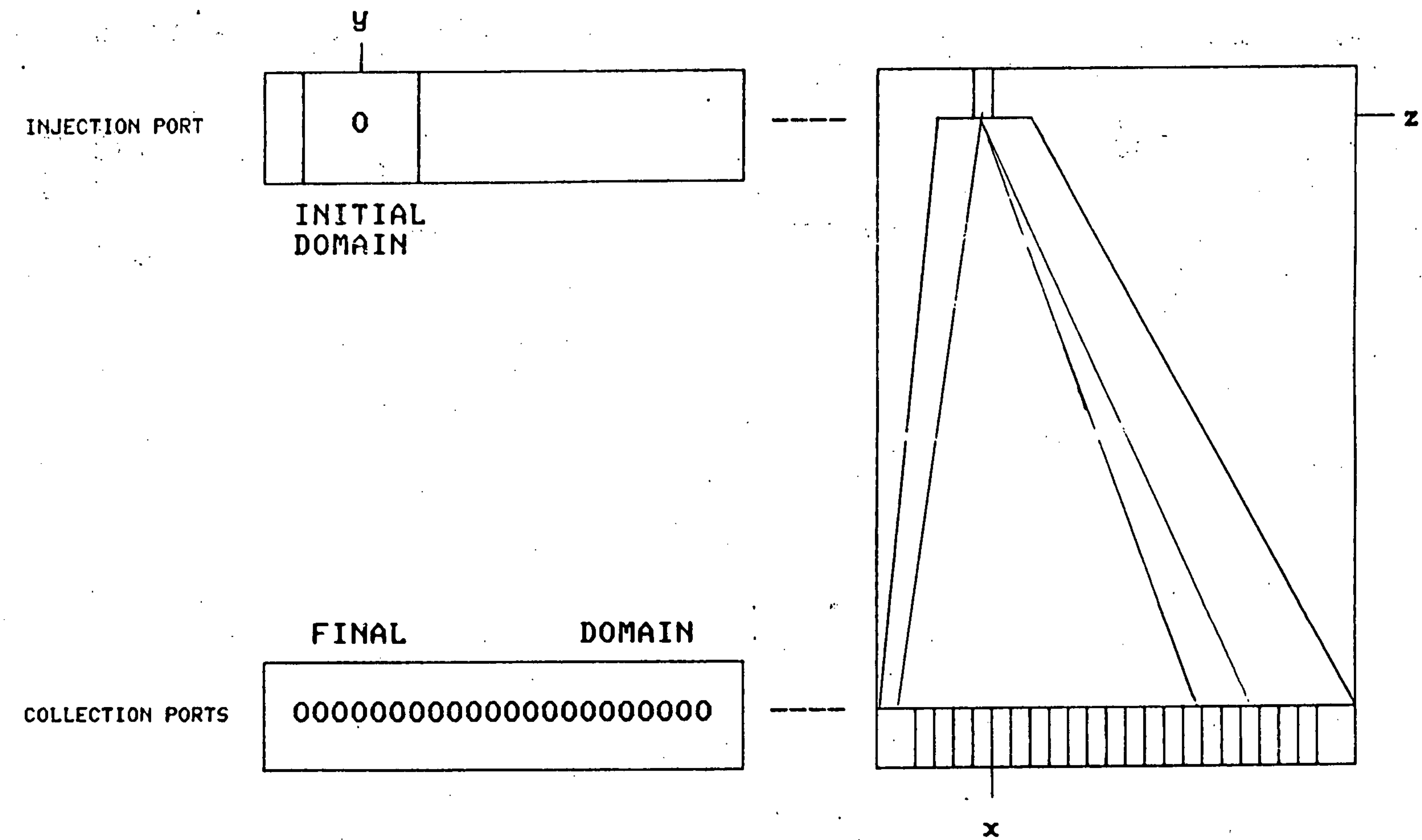
CHART NO.: DESCRIPTION- 19	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 10, 1984

COMPUTATIONAL DOMAIN (continued)



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ORGANIZATION: RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 20	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14, 1984

BOUNDARY CONDITIONS

- y BOUNDARIES: ZERO FLUX OF EVERY RADICAL
- ISOELECTRIC FOCUSING
  NO FLUX AT EITHER z BOUNDARY
- ALL OTHER CASES
  CONCENTRATIONS IMPOSED WHEN MEAN ION MOTION IS INTO THE DOMAIN
  ZERO DERIVATIVE (PASSIVE) WHEN MEAN ION MOTION IS OUT OF THE DOMAIN

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CHART NO.: RESULTS- 21	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14,1984

OUTPUT OPTIONS

- ➤ NUMERICAL DIAGNOSTICS
- ➤ GRAPHICS OUTPUT
  - ● PRINTER
  - ● TEKTRONIX (1D AND 2D)
  - ● (MOVIES)
- ➤ GRAPHICS PLOTS ARE AVAILABLE FOR THE FOLLOWING VARIABLES
  - ● GENERAL VARIABLES
    - pH = – log(H)
    - CONDUCTIVITY (MHO/CM)
    - DISTURBANCE VOLTAGE
    - CURRENT LINES (AMPS/CM)
    - ELECTRIC FIELD (VOLTS/CM)
    - TRANSVERSE ELECTRIC FIELD (VOLTS/CM)
    - DIFFUSION CURRENT POTENTIAL (AMPS/CM)
  - ● FOR EACH RADICAL TYPE
    - MOLAR CONCENTRATION
    - MEAN IONISATION
    - MEAN SQUARE IONISATION
    - CHARGE MOLARITY
    - CONDUCTIVITY (MHO/CM)
    - CONCENTRATION CHANGE
    - VELOCITY FUNCTION (CM/SEC)

14-FEB-84 07:35

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 22	ELECTROPHORESIS MODELING INPUT DATA PAGE	DATE: JANUARY 18, 1984

CELLULOSE ACETATE A/8.8(2)/0.75X/MIX

PROBLEM PARAMETERS

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Z MESH                          Y MESH                      SAMPLE                        WATER MOBILITIES         SIDE BOUNDARY CONDITIONS
                                                            ELECTRIC FIELD                BOUNDARY FLOW     1/2/3 FOR BUFFER/SAMPLE/NO-FLUX
ZBL   =   -1.0000000            YT    =   1.0000000         YSAMP =   0.0000000           UH  =   0.0036000        ILEFT  = 1
ZBR   =    1.0000000            YB    =   0.0000000         RSAMP =   0.1000000           UOH =   0.0020000        IRIGHT = 1
ZDL   =    0.0000000            DYRAT =   4.0000000         PSAMP =   1.0000000           UWE =   0.0000000
ZDR   =    0.0000000
DZRAT =    4.0000000                                        EZERO =  -10.0000000          UB  =   1.0000000
```

SPECIES	BUFFER MOLARITY	SAMPLE MOLARITY	SINGLE ION MOBILITY	IONISATION DEFINITION CONSTANTS	N			N			N			N		
SODIUM	0.00190000	0.00570000	0.00052700	-3.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BARBITURATE	0.00228000	0.00684000	0.00036000	-1.00	7.85	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEMOGLOBIN A	0.00000000	0.00130000	0.00001000	36.09	25.74	3.39	7.86	17.32	6.82	10.45	11.40	6.97	6.99	12.65	4.99	4.79

METHOD PARAMETERS

```
TIME STEPS          ADVECTION           FIXING CONTROLS      FIXING AMPLITUDES     POISSON METHOD
NSTEP =  120        CUPUND =  0.050     FIXCZ = T            BETCA =  0.500        NPITER =   10
TSTEP =   1.00      THZFX  =  0.167     FIXCY = T            BETCD =  0.500        PEXTRP =  0.500
```

OUTPUT PARAMETERS

```
DIRECT ACCESS READ & WRITE SEGMENTS       WRITE STEP BEGINNING & INCREMENT     DIAGNOSTIC FREQUENCY    CONTOUR LINES
ISEGR =   0   ISEGU =   1                   IBEGDA =   0    IINCDA -9900        NDIAG =  0         NCLP =  0  NCLI =  0
(0: ANALYTIC. -1: AFTER PRIOR CASE)         (ZERO MEANS NSTEP)   YPLB =  0.00   YPLT =  0.40        NCOPIES =  1
```

VARIABLE	ISTEP BEGIN & INCREMENT FOR PRINTER DIAGNOSTICS PHYSICAL	CONTOUR	INTEGER	CONTOUR	PRINT NUMBERS		RANGES FOR I AND K IB	IE	II	KB	KE	KI	PLOTTER IDAOUT BEGIN & INCREMENT PHYSICAL		INTEGER		INCR
PH	0	40	9903	9904	0	-12	-1	82	1	2	2	-1	1	9914	9915	9916	0.0
SIGMA	0	40	9903	9904	0	-12	-1	82	1	2	2	-1	1	9914	9915	9916	0.0
PHI	0	40	9903	9904	0	-12	-1	82	1	2	2	-1	1	9914	9915	9916	0.0
CURRENT	0	40	9903	9904	0	-12	-1	81	1	2	2	-1	1	9914	9915	9916	0.0
EZ	0	40	9903	9904	0	-12	-1	81	1	2	2	-1	1	9914	9915	9916	0.0
EY	0	40	9903	9904	0	-12	-1	81	1	2	2	-1	1	9914	9915	9916	0.0
SODIUM																	
CONC	0	40	9903	9904	0	-12	-1	82	1	2	2	-1	1	9914	9915	9916	0.0
MEAN ION	9901	9902	9903	9904	0	-12	-1	82	1	2	2	-1	9913	9914	9915	9916	0.0
MEAN SQU	9901	9902	9903	9904	0	-12	-1	82	1	2	2	-1	9913	9914	9915	9916	0.0
CHARGE	9901	9902	9903	9904	0	-12	-1	82	1	2	2	-1	1	9914	9915	9916	0.0
SIGMA	0	40	9903	9904	0	-12	-1	82	1	2	2	-1	1	9914	9915	9916	0.0
DCONC	0	40	9903	9904	0	-12	-1	82	1	2	2	-1	1	9914	9915	9916	0.0
VELOCITY	0	40	9903	9904	0	-12	-1	82	1	2	2	-1	1	9914	9915	9916	0.0

18-JAN-84 07:44

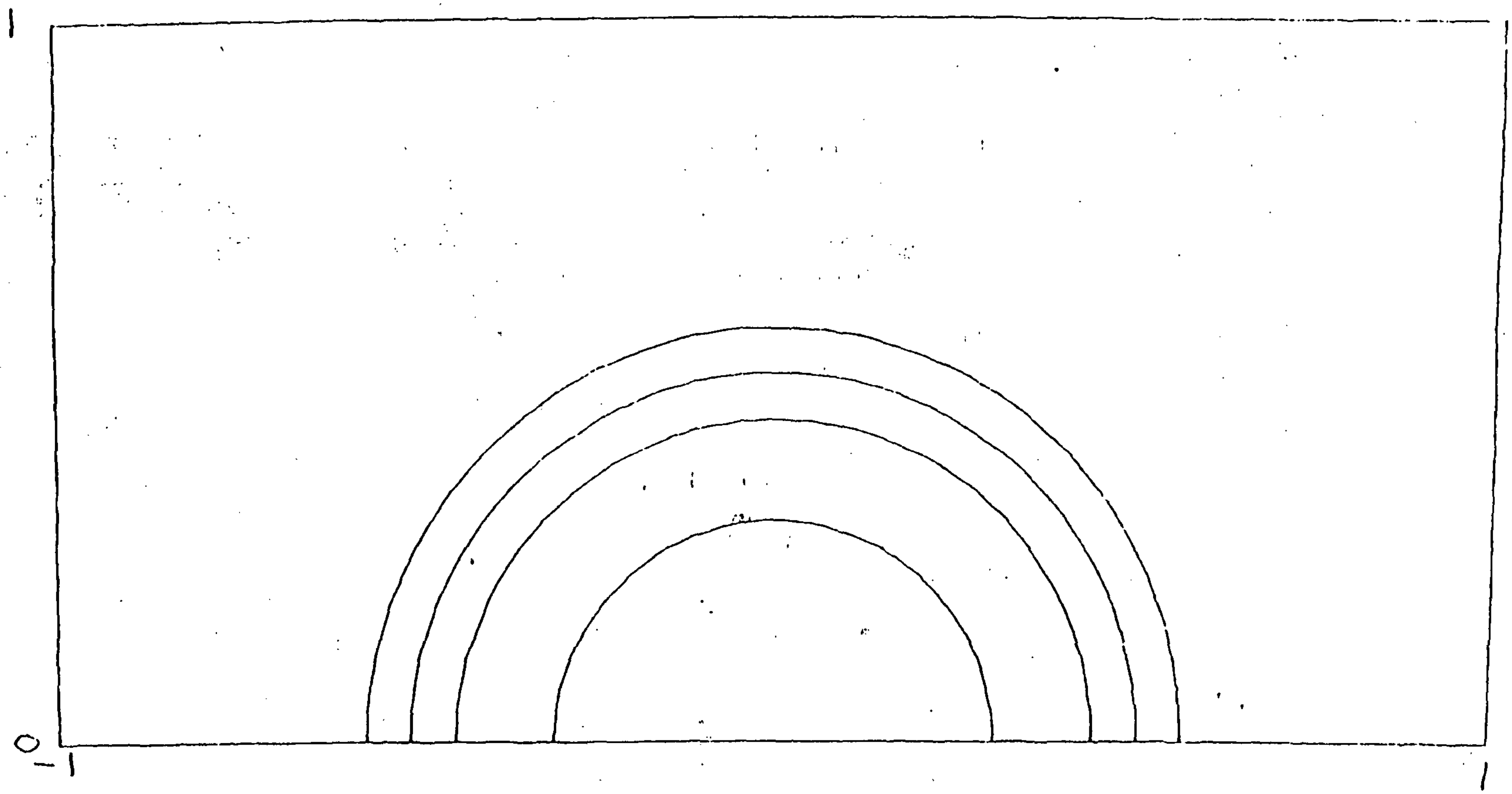
ORGANIZATION: RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 23	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14,1984

ANALYTIC VALIDATIONS

- pH AND CONDUCTIVITY COMPUTATION
  - pH AGREES EXACTLY WITH MEASUREMENT AND THEORY FOR CASES ANALYZED
  - CONDUCTIVITY AGREES WITH MEASUREMENTS ONLY FOR LOW CONCENTRATIONS. THE MODEL CONDUCTIVITY IS LINEAR IN CONCENTRATION.
- ELECTRIC FIELD AND CURRENT CALCULATION
  - AGREEMENT WITH THEORY FOR SIMPLE CASES.
  - AGREEMENT OF CURRENT AND POTENTIAL METHODS.
  - INTERNAL CONSISTENCY.
- EVOLUTION OF RADICAL CONCENTRATIONS
  - NO CHANGE IN CIRCULAR SAMPLE UNDER
    - ZERO FIELD, MOVING DOMAIN
    - WEAK SAMPLE, UNIFORM FIELD
  - CORRECT SPREADING OF CIRCULAR GAUSSIAN SAMPLE UNDER DIFFUSION ALONE
  - AGREEMENT WITH ANALYTIC SOLUTION FOR SEPARATION OF THREE HEMOGLOBIN TYPES AT LOW CONCENTRATIONS.

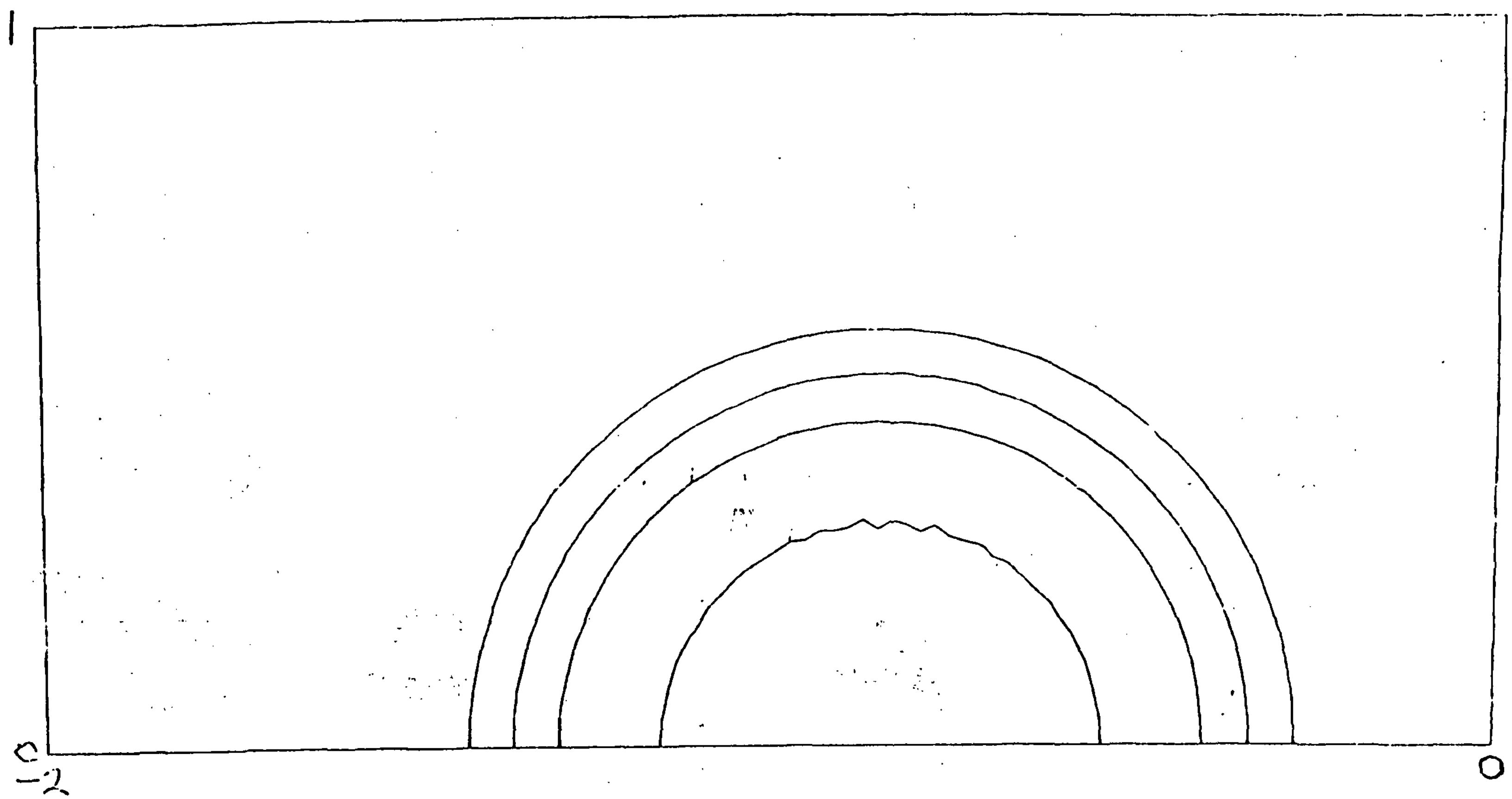
14-FEB-84 07:36

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 24	ELECTROPHORESIS MODELING VALIDATION RESULTS	DATE: JANUARY 18, 1984



MOLAR CONCENTRATION FOR HEMOGLOBIN A
WEAK HEMOGLOBIN TEST
MAXIMUM = 1.27658E-07
MINIMUM = -2.37528E-15
INCREMENT = 3.00000E-08
TIME = 1.00000E-02

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 25	ELECTROPHORESIS MODELING VALIDATION RESULTS	DATE: JANUARY 18, 1984



MOLAR CONCENTRATION FOR HEMOGLOBIN A
WEAK HEMOGLOBIN TEST/MOVING WALL
MAXIMUM = 1.27742E-07
MINIMUM = -4.07884E-16
INCREMENT = 3.00000E-08
TIME = 40.000

CELLULOSE ACETATE FILM EXPERIMENTS

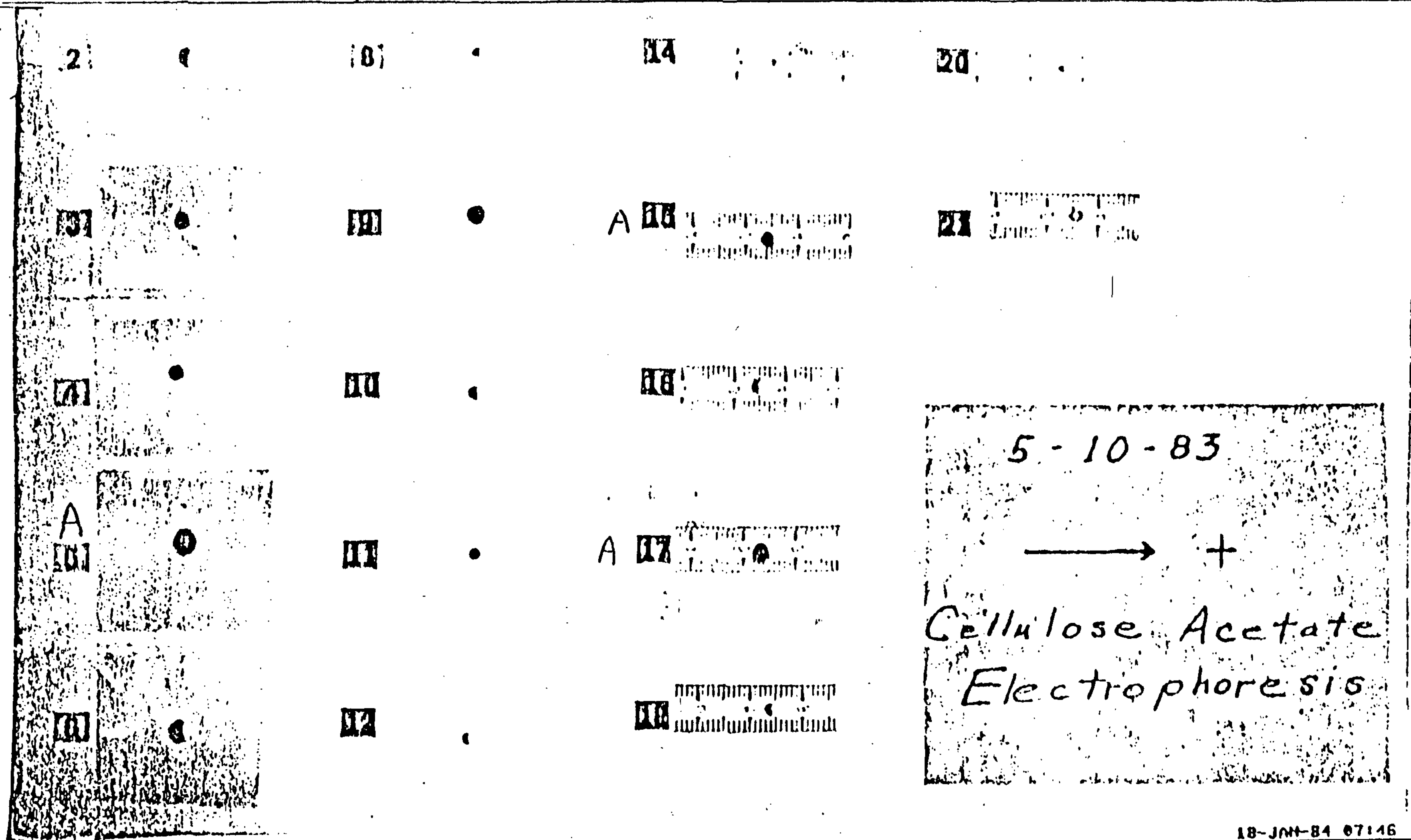
HEMOGLOBIN TESTS WERE PERFORMED IN MAY, 1983, USING SIX DIFFERENT SAMPLES AND FOUR DIFFERENT BARBITOL BUFFERS.

WE COULD SIMULATE ONLY FOUR OF THE SAMPLES DUE TO UNCERTAINTY OF CONTENT.
THIS INVOLVED A TOTAL OF EIGHT DISTINCT TESTS.
PLOTS OF THE HEMOGLOBIN DISTRIBUTIONS CAN BE COMPARED WITH PHOTOGRAPHS.

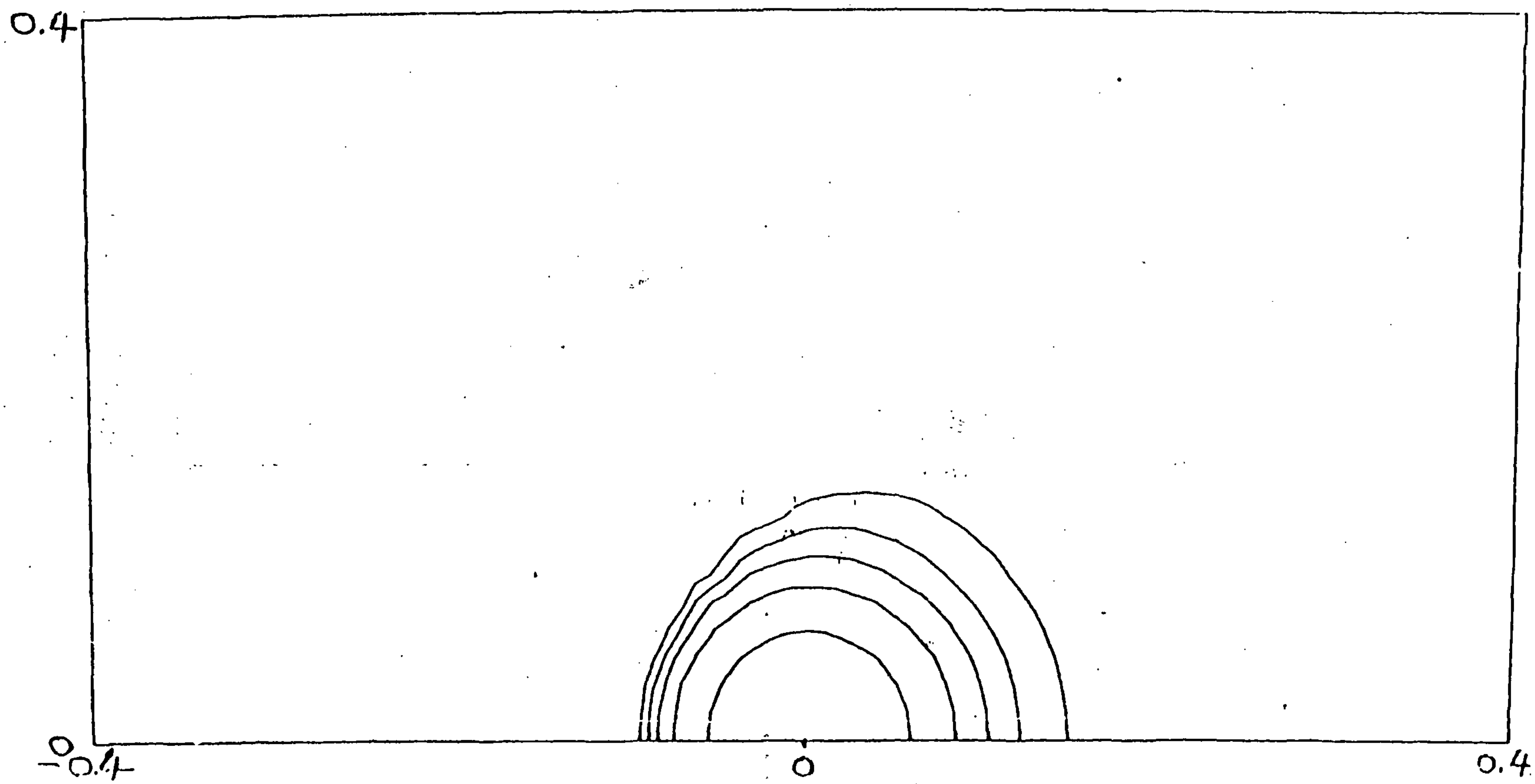
THE COMPARISONS ARE REASONABLY GOOD

WE ATTRIBUTE THE DIFFERENCES TO THE FOLLOWING CAUSES
- MODEL IS POOR FOR HIGH CONCENTRATIONS
- METHOD OF APPLYING SAMPLE TO THE FILM CAUSED MIXING WITH BUFFER
- POSSIBLE EFFECTS OF OTHER COMPONENTS IN THE SAMPLE AND BUFFER
- POSSIBLE OTHER DEFICIENCIES IN THE MODEL

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER ELECTROPHORESIS MODELING CELLULOSE ACETATE FILM EXPERIMENTS	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 27		DATE: JANUARY 18, 1984



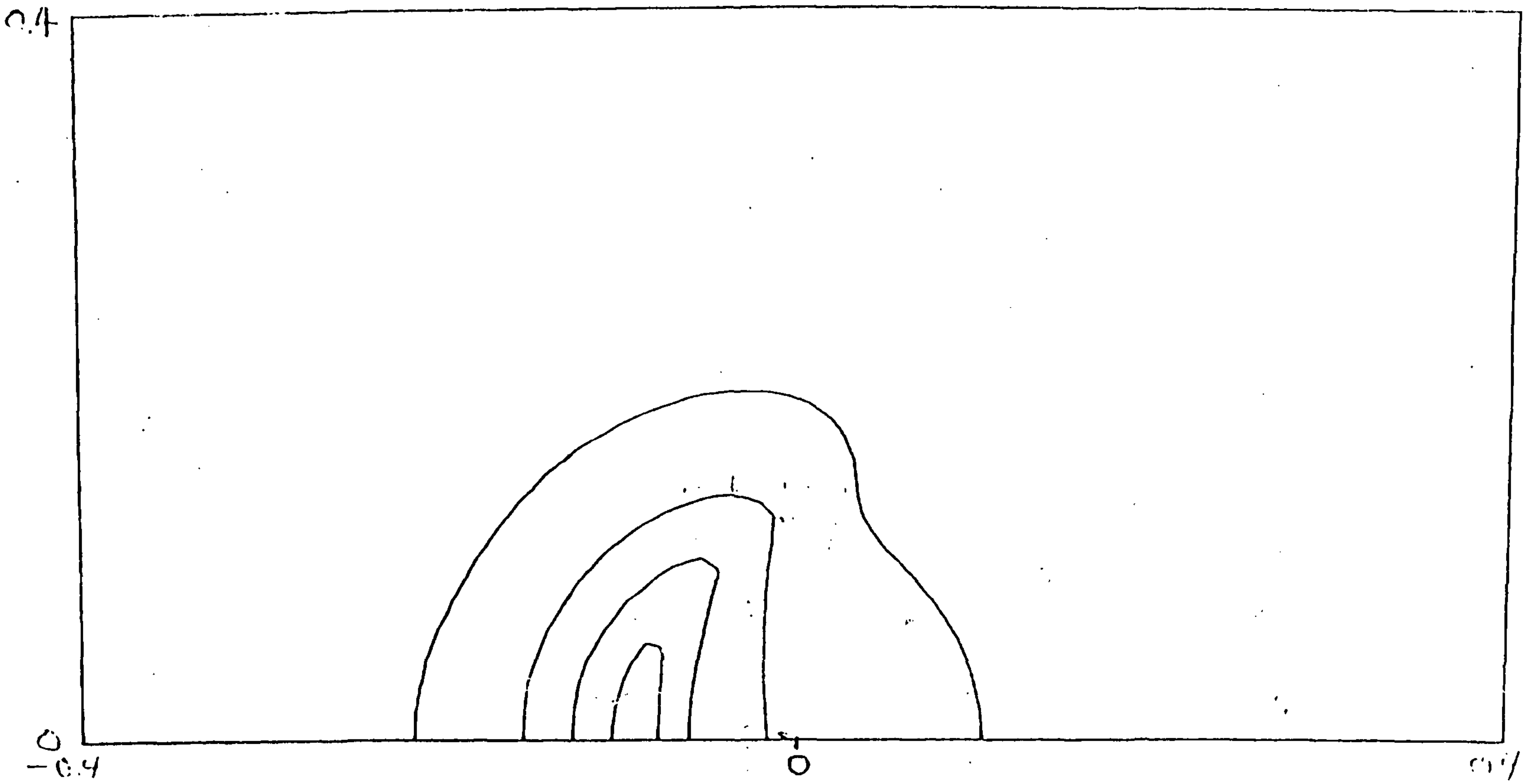
ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 28	ELECTROPHORESIS MODELING CELLULOSE ACETATE FILM EXPERIMENTS	DATE: JANUARY 18, 1984



MOLAR CONCENTRATION FOR HEMOGLOBIN A
CELLULOSE ACETATE A/8.8(2)/0.75X/MIX
MAXIMUM = 1.14081E-03
MINIMUM = -4.26128E-06
INCREMENT = 2.00000E-04
TIME = 120.00

18-JAN-84 07:46

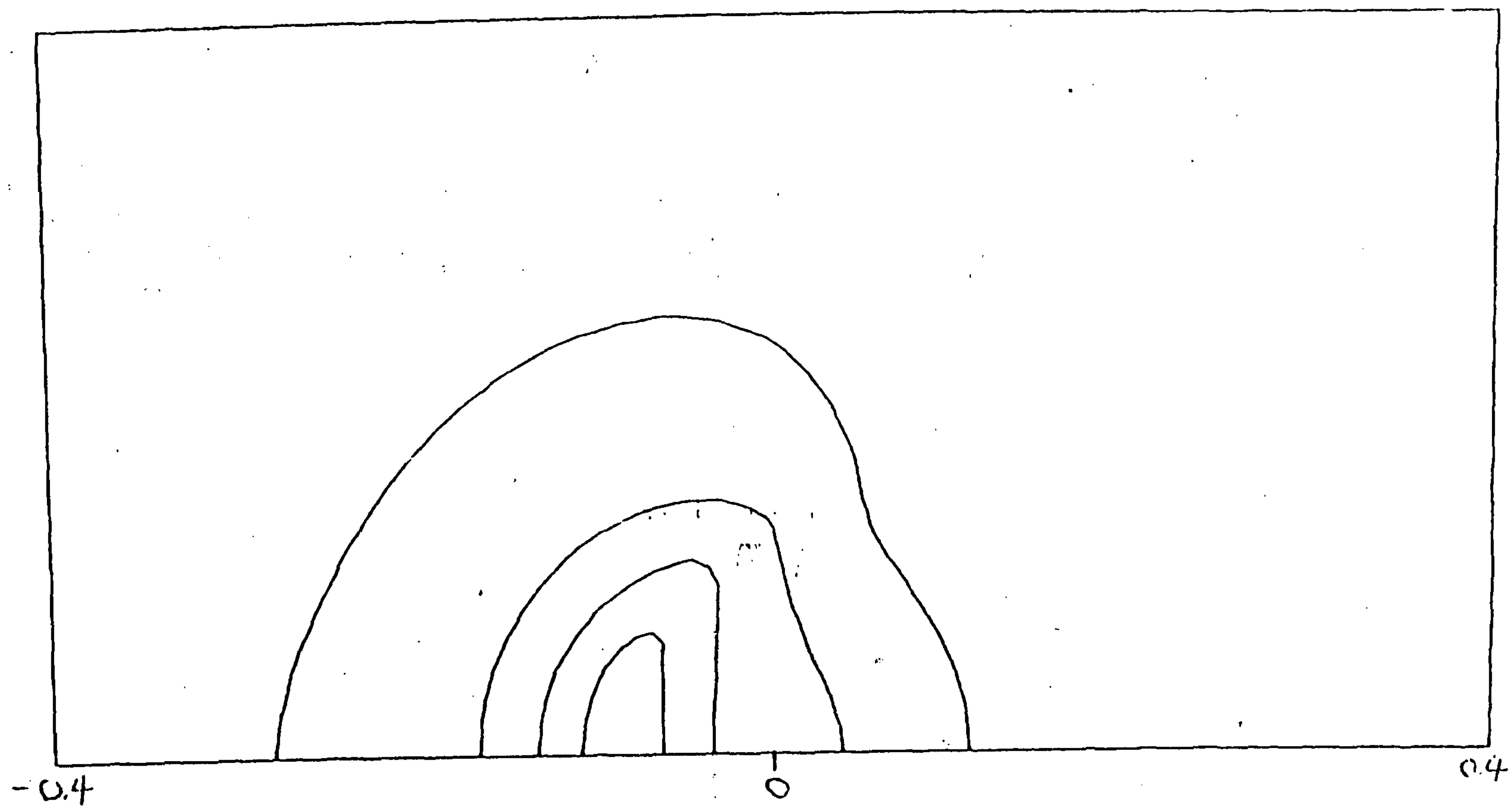
ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 29	ELECTROPHORESIS MODELING CELLULOSE ACETATE FILM EXPERIMENTS	DATE: JANUARY 18, 1984



MOLAR CONCENTRATION FOR BARBITURATE
CELLULOSE ACETATE A/8.8(2)/0.75X/MIX
MAXIMUM - 1.34139E-02
MINIMUM - 5.75363E-04
INCREMENT - 3.00000E-03
TIME - 120.00

18-JAN-84 07:46

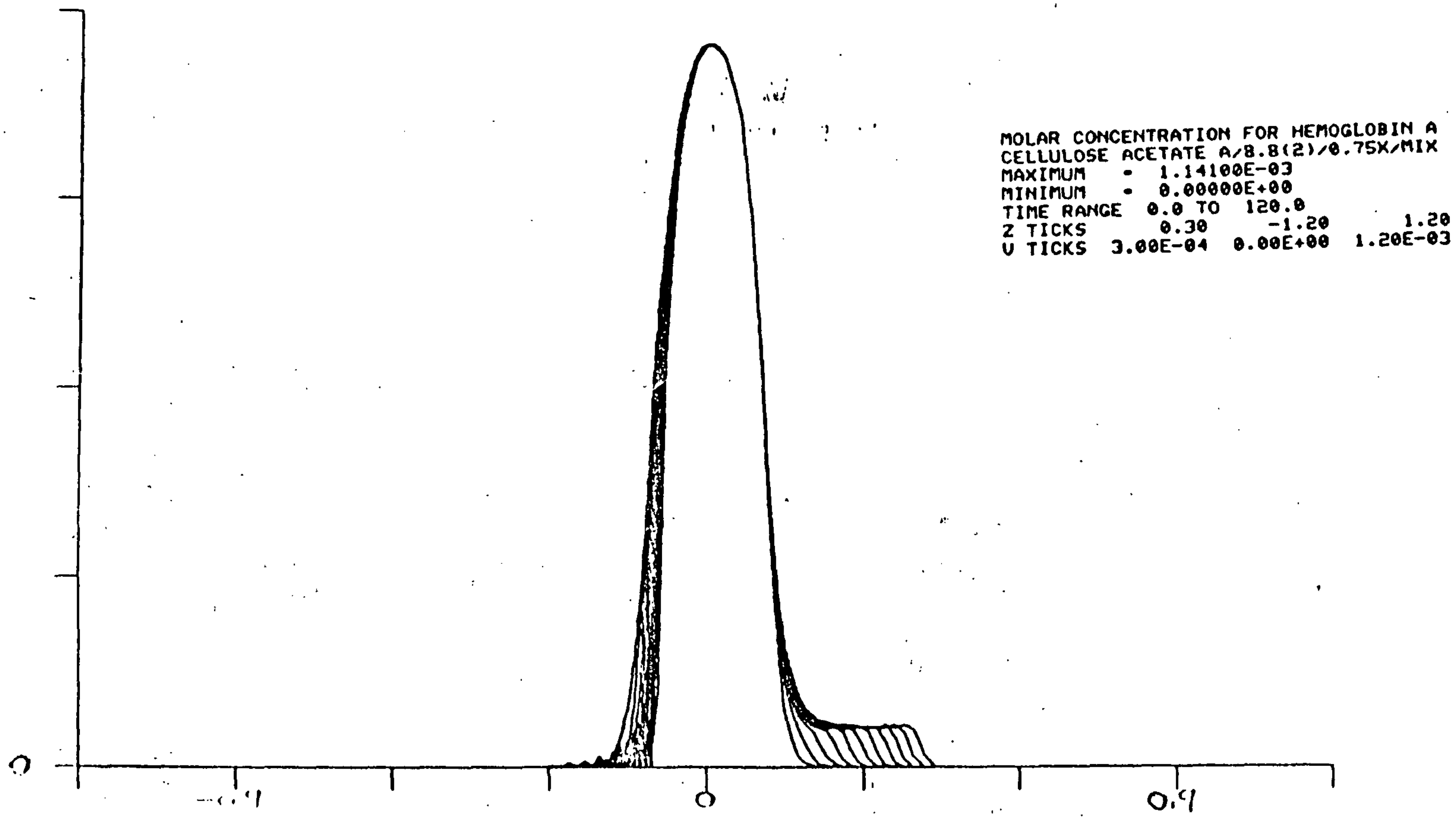
ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 30	ELECTROPHORESIS MODELING CELLULOSE ACETATE FILM EXPERIMENTS	DATE: JANUARY 18, 1984



MOLAR CONCENTRATION FOR SODIUM
CELLULOSE ACETATE A/8.8(2)/0.75X/MIX
MAXIMUM • 9.46580E-03
MINIMUM • 5.80182E-04
INCREMENT • 2.00000E-03
TIME • 120.00

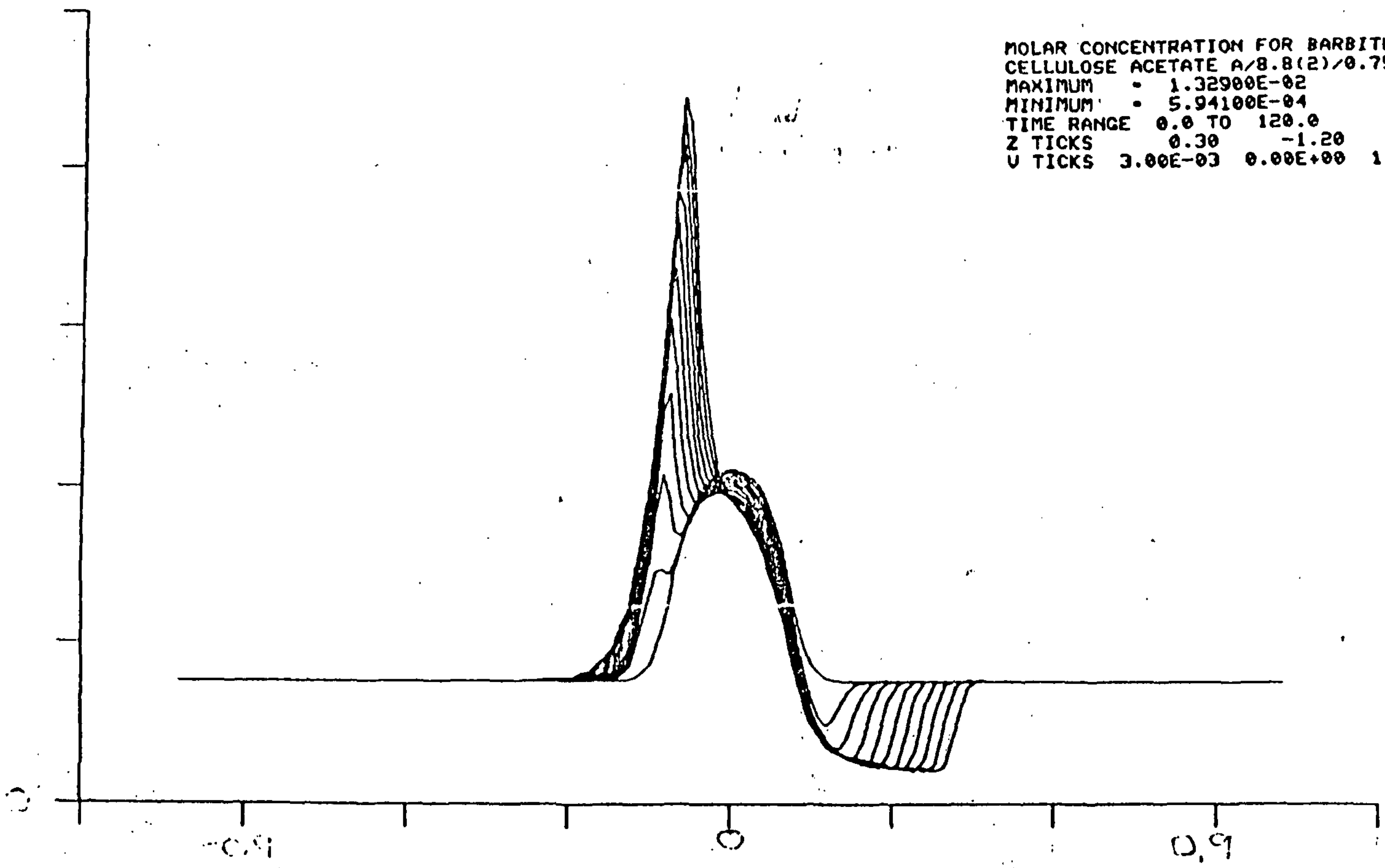
18-JAN-84 07:46

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 31	ELECTROPHORESIS MODELING CELLULOSE ACETATE FILM EXPERIMENTS	DATE: JANUARY 18, 1984



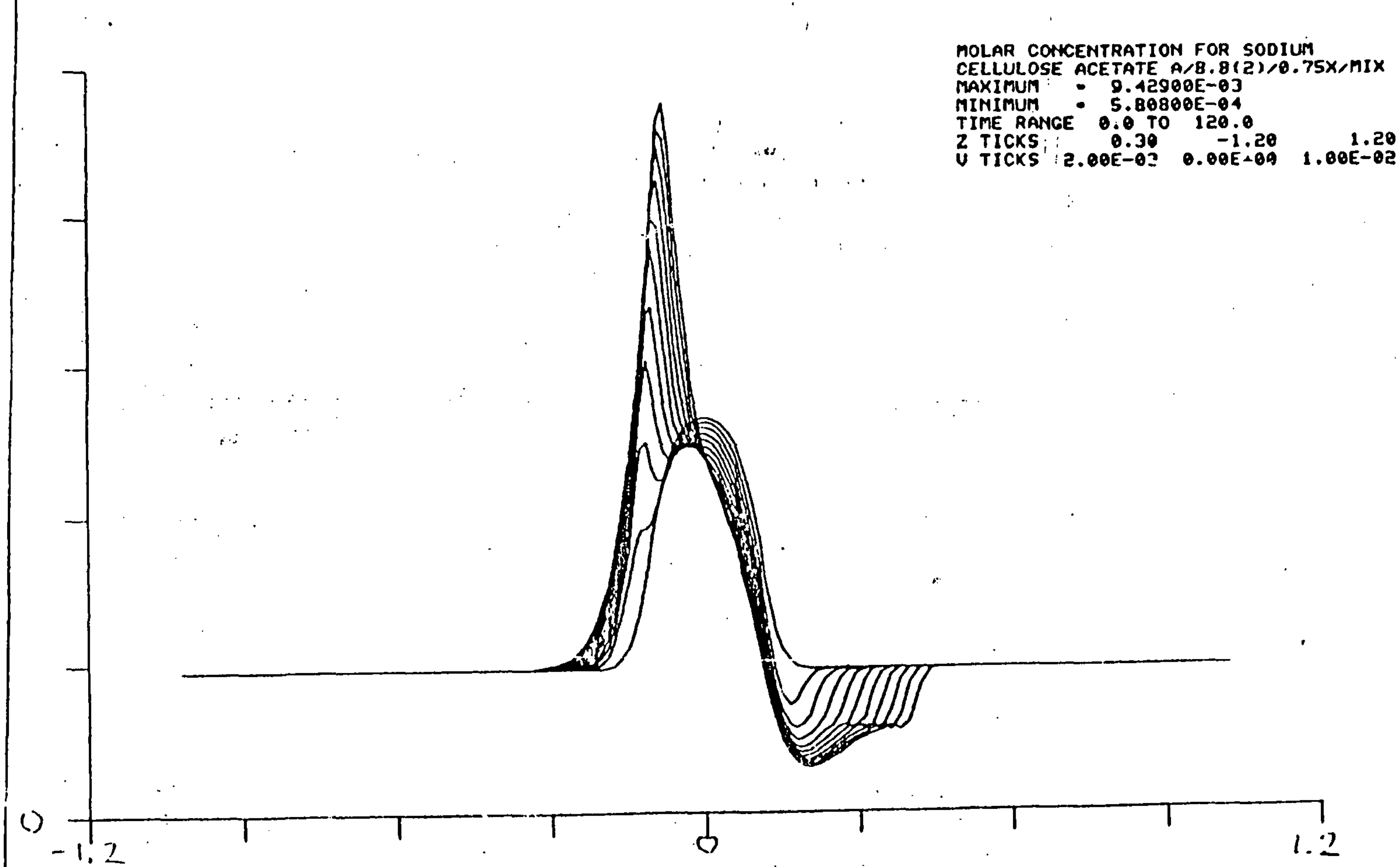
18-JAN-84 07:47

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 32	ELECTROPHORESIS MODELING CELLULOSE ACETATE FILM EXPERIMENTS	DATE: JANUARY 18, 1984



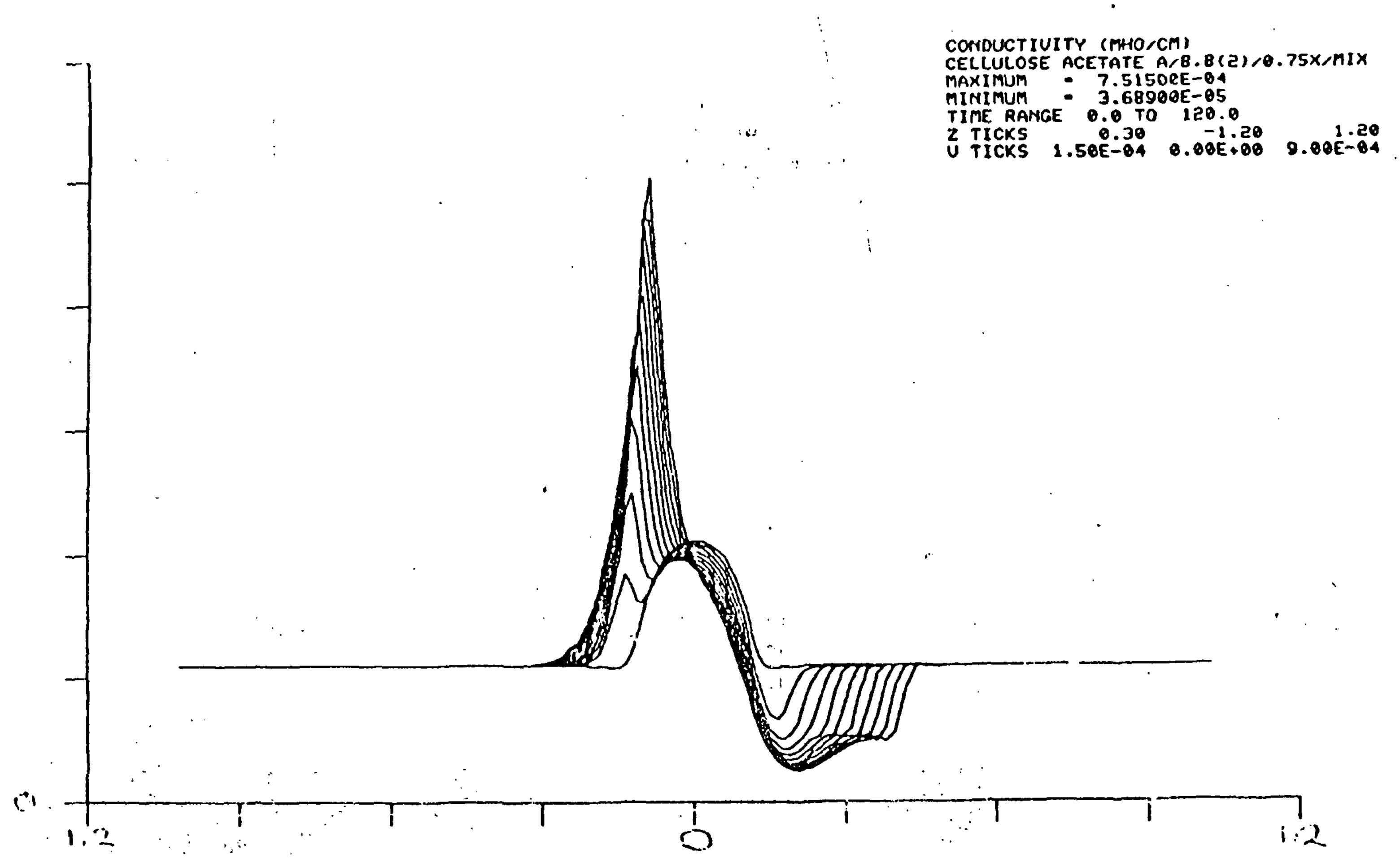
18-JAN-84 07:47

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 33	ELECTROPHORESIS MODELING CELLULOSE ACETATE FILM EXPERIMENTS	DATE: JANUARY 18, 1984

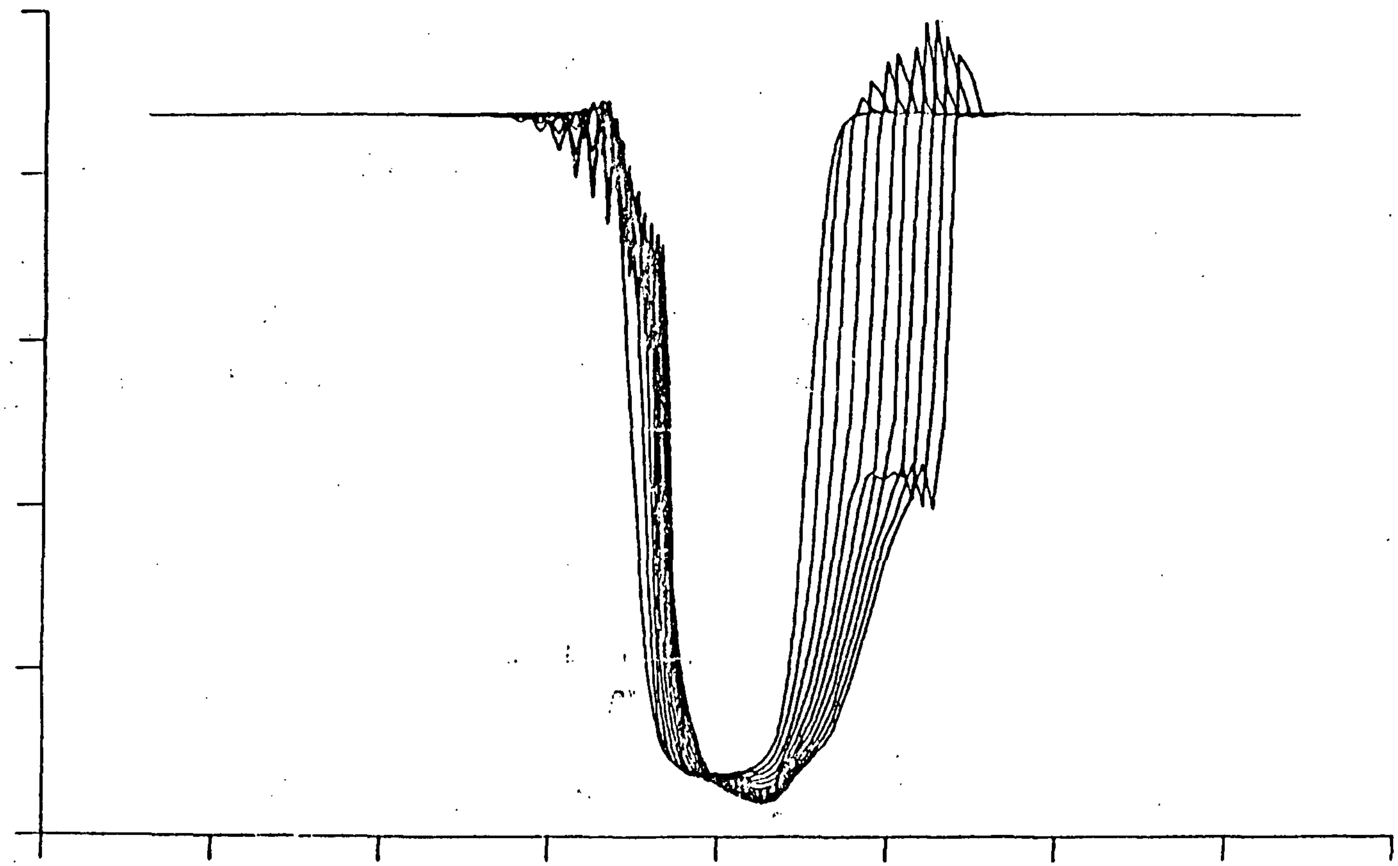


18-JAN-84 07:47

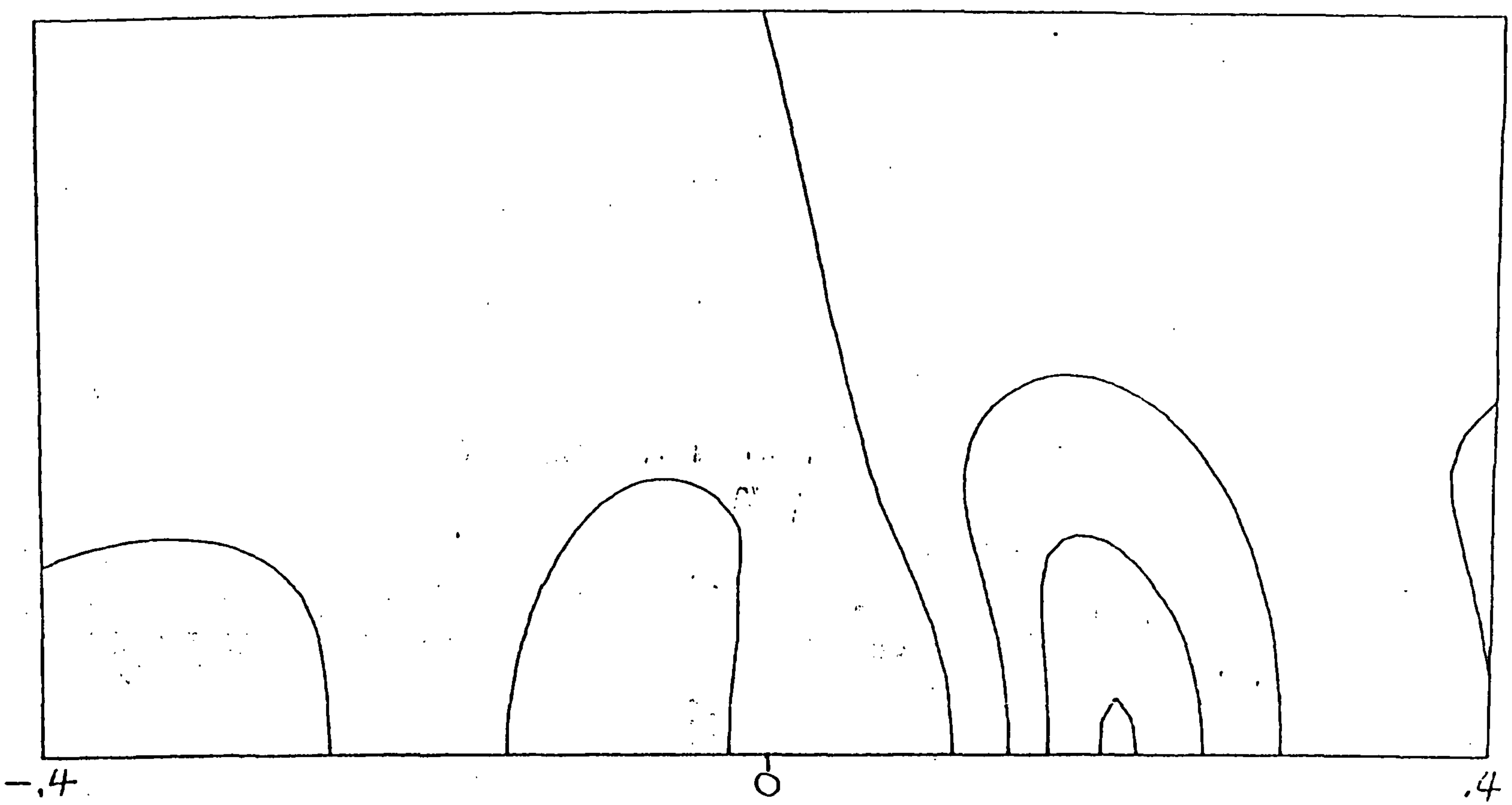
ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 34	ELECTROPHORESIS MODELING CELLULOSE ACETATE FILM EXPERIMENTS	DATE: JANUARY 18, 1984



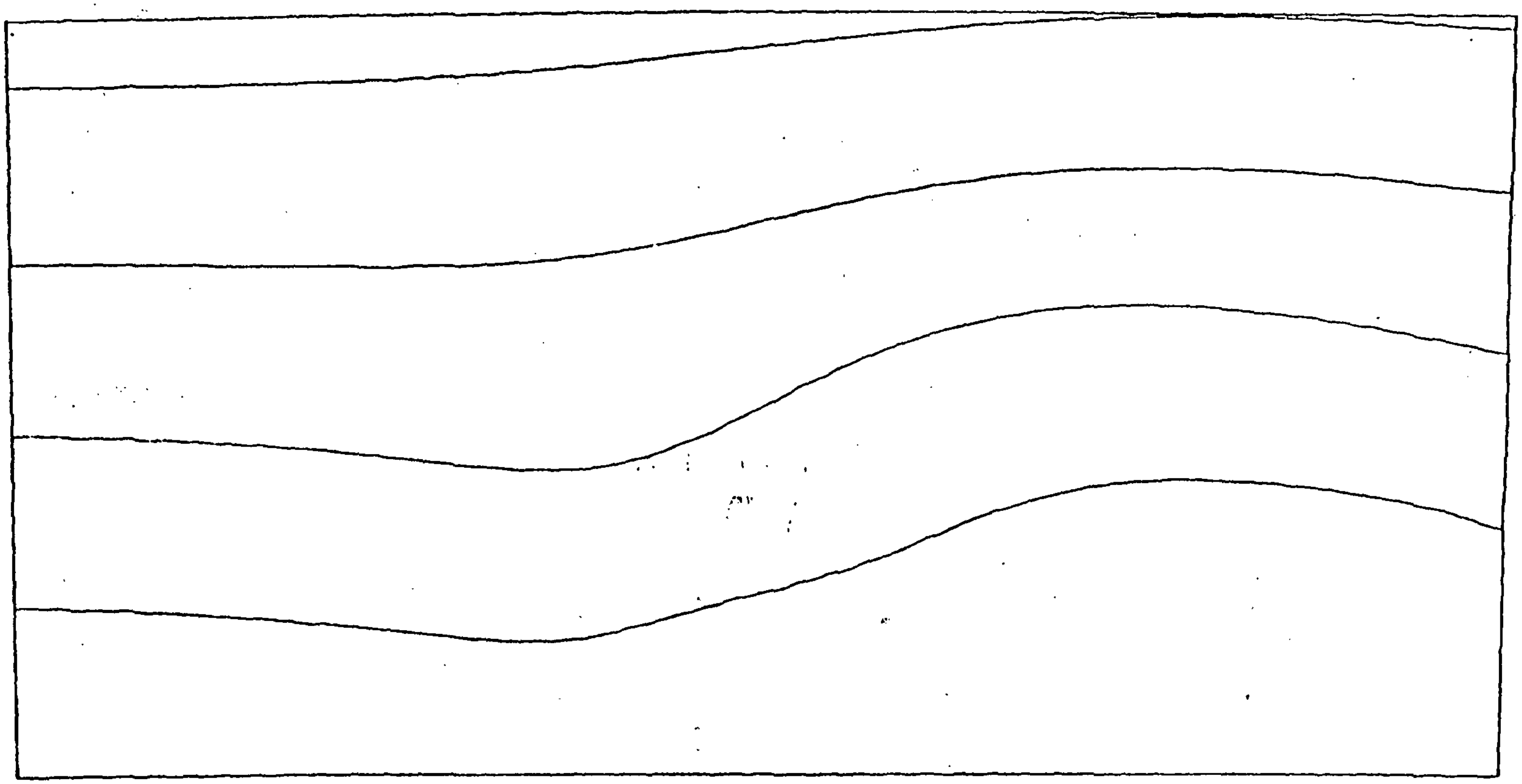
18-JAN-84 07:47



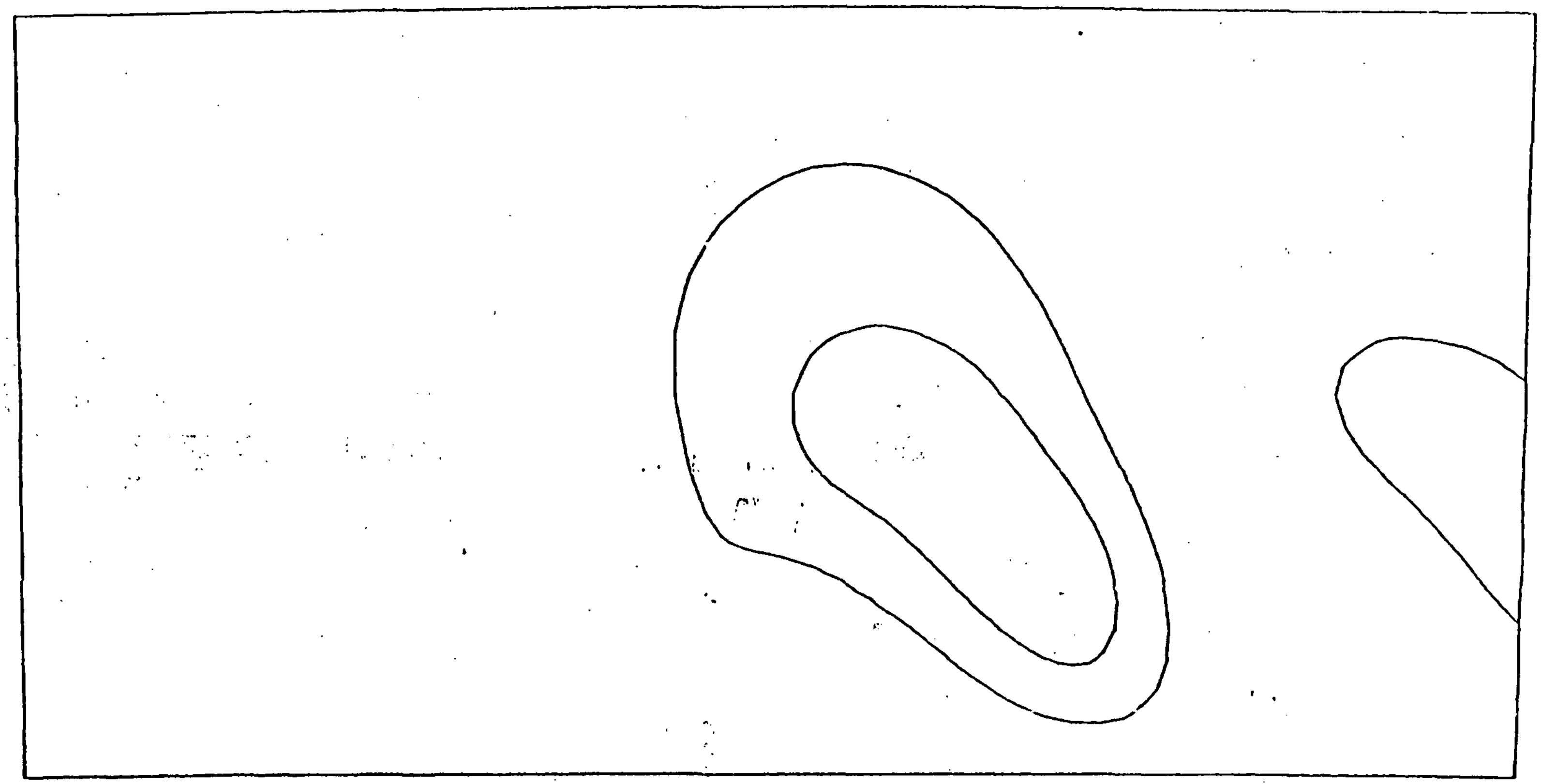
pH = - LOG10(H)
CELLULOSE ACETATE A/8.8(2)/0.75X/MIX
MAXIMUM - 8.7770
MINIMUM - 6.8810
TIME RANGE 0.0 TO 120.0
Z TICKS 0.30 -1.20 1.20
V TICKS 4.00E-01 6.80E+00 8.80E+00



ELECTRIC FIELD (V/CM)
CELLULOSE ACETATE A/8.8(2)/0.75X/MIX
MAXIMUM - -2.8429
MINIMUM - -25.445
INCREMENT - 5.0000
TIME - 120.00



CURRENT LINES (AMPS/CM)
CELLULOSE ACETATE A/8.8(2)/0.75X/MIX
MAXIMUM - 6.44569E-11
MINIMUM - -6.57587E-04
INCREMENT - 1.50000E-04
TIME - 120.00



TRANVERSE ELECTRIC FIELD (V/CM)
CELLULOSE ACETATE A/8.8(2)/0.75X/MIX
MAXIMUM = 2.8301
MINIMUM = -5.8856
INCREMENT = 2.0000
TIME = 120.00

ORGANIZATION: RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 35	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14, 1984

CONTINUOUS FLOW ELECTROPHORESIS

TESTS PERFORMED TO DATE HAVE INVOLVED WEAK CONCENTRATIONS OF HEMOGLOBIN:

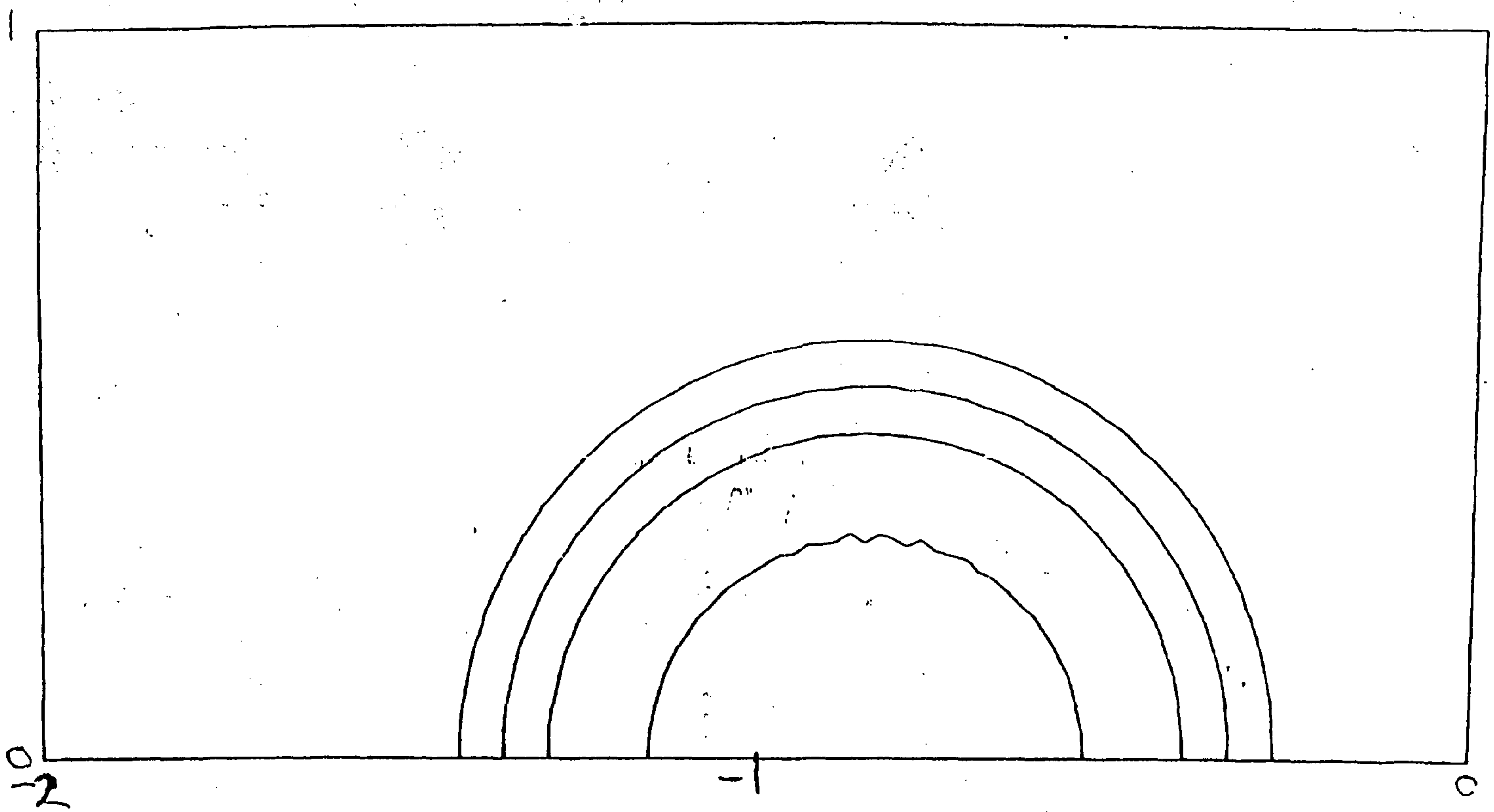
- MOVING WALL – STRAIGHT ADVECTION WITH NO SHAPE CHANGE
- CFE – MORE MOTION AT EDGES, LEADING TO CRESCENT SHAPE
- CFE WITH NEGATIVE ELECTRO-OSMOSIS – STRONGER CRESCENT
- CFE WITH POSITIVE ELECTRO-OSMOSIS – NO SHAPE CHANGE.

THIS ALL AGREES WITH ANALYTIC SOLUTIONS.

THE TIME STEPS ARE EFFECTIVELY INFINITE AT THE EDGES, SINCE THE MEAN FLOW DOWN THE COLUMN IS ZERO.

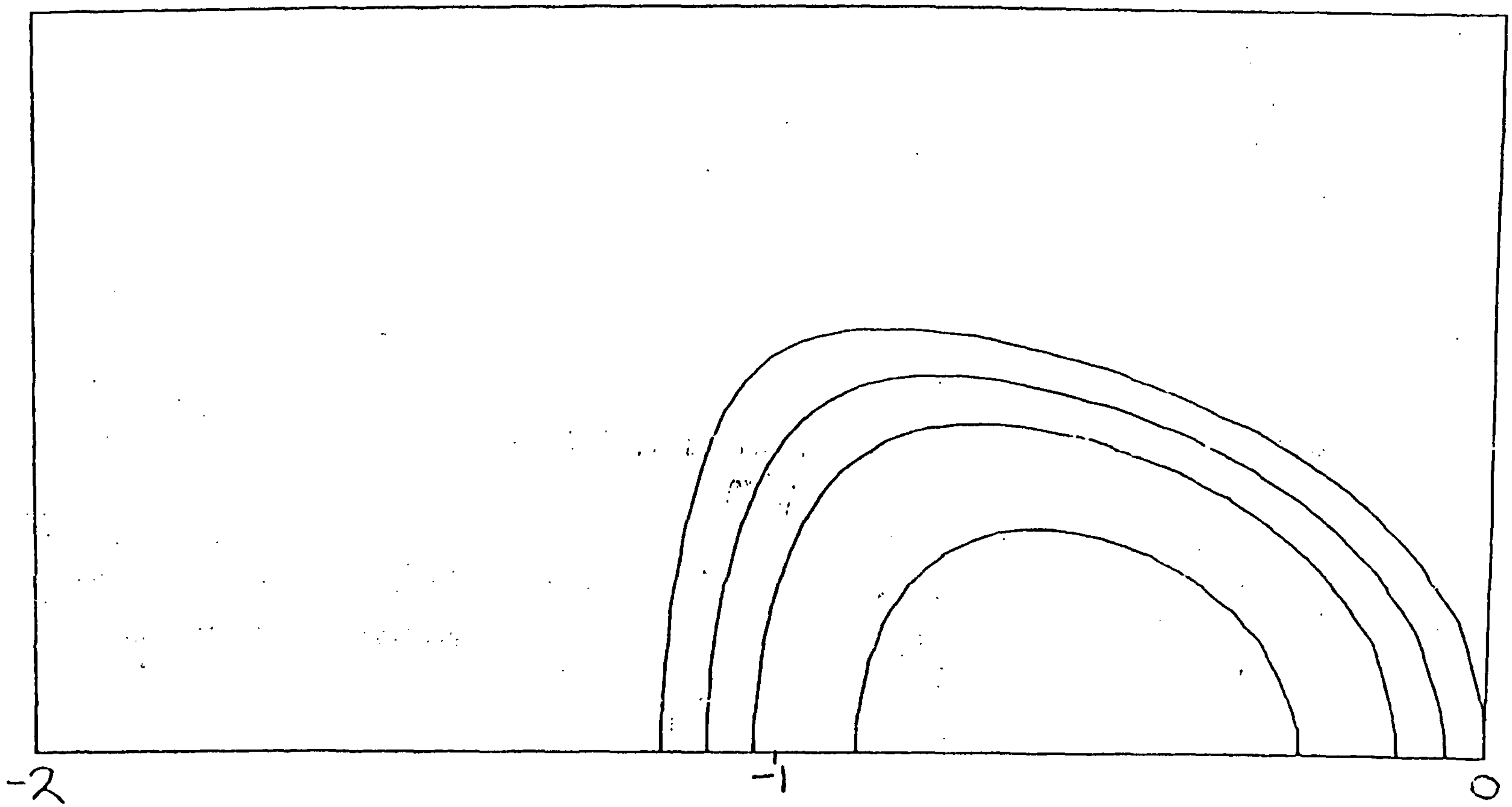
WE HAVE NOT EXPERIENCED INSTABILITY PROBLEMS. THIS IS DUE TO OUR USE OF IMPLICIT METHODS.

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 36	ELECTROPHORESIS MODELING CFE TEST RESULTS	DATE: JANUARY 18, 1984



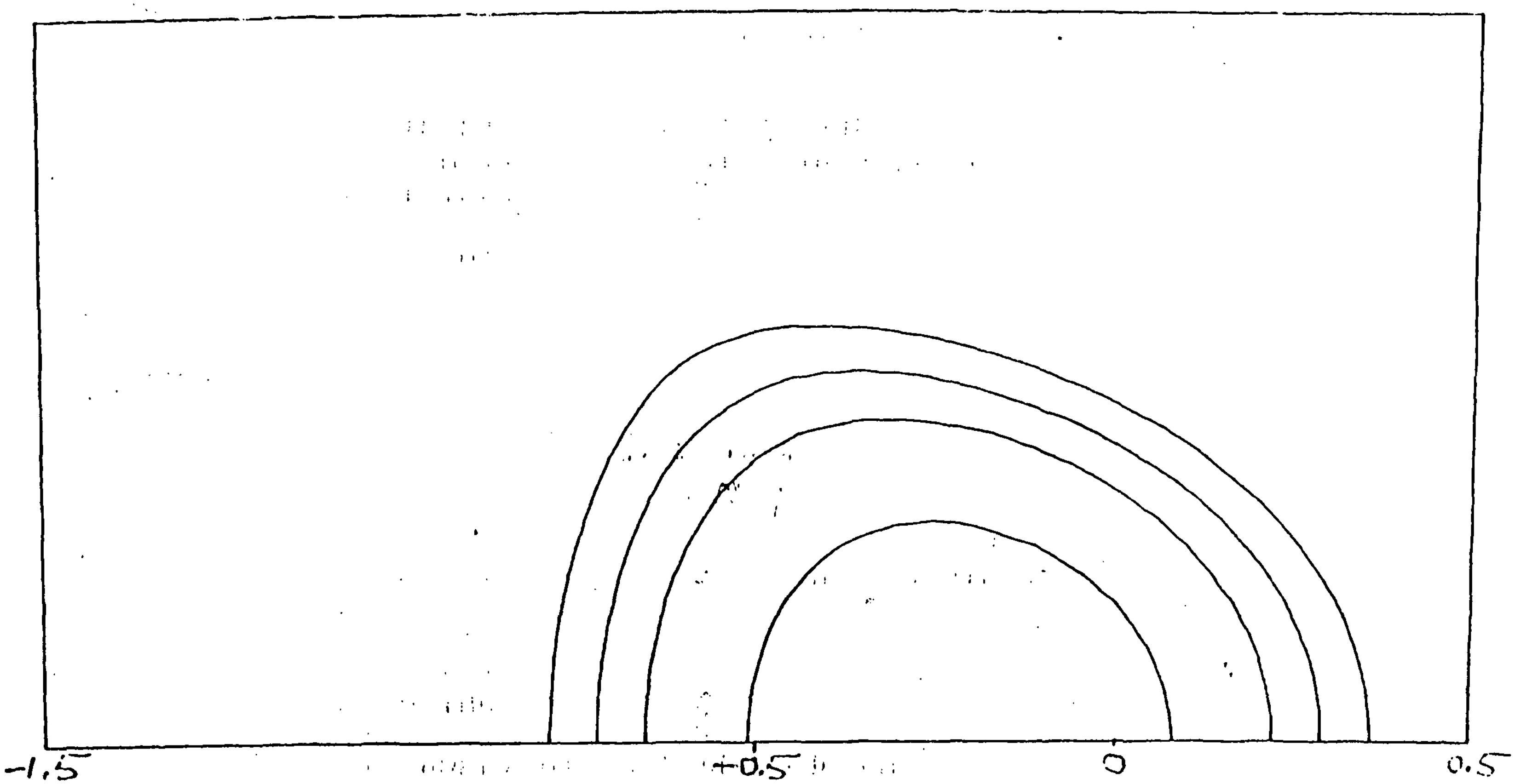
MOLAR CONCENTRATION FOR HEMOGLOBIN A
WEAK HEMOGLOBIN TEST/MOVING WALL
MAXIMUM = 1.27742E-07
MINIMUM = -4.07884E-16
INCREMENT = 3.00000E-08
TIME = 40.000

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 37	ELECTROPHORESIS MODELING CFE TEST RESULTS	DATE: JANUARY 18, 1984



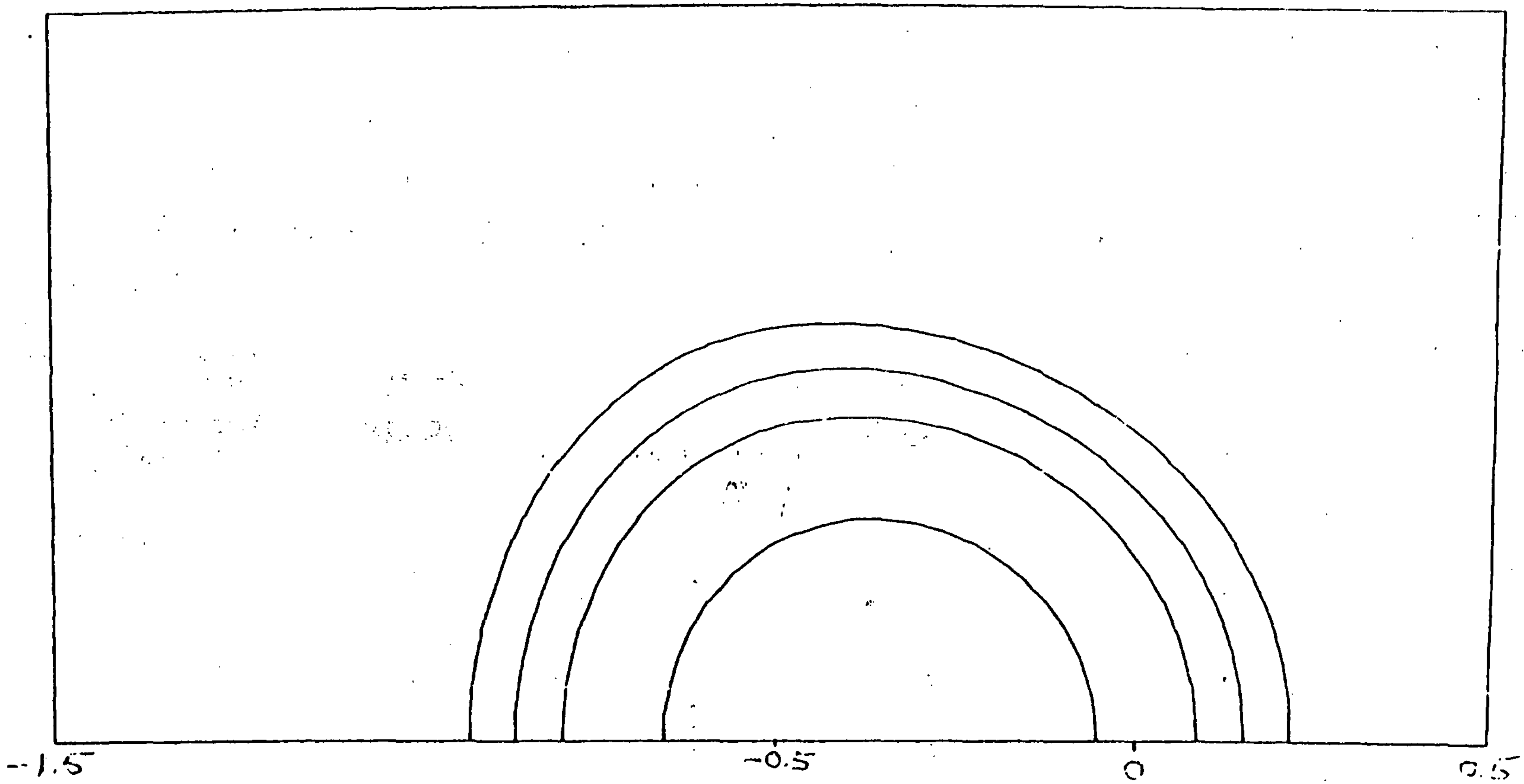
MOLAR CONCENTRATION FOR HEMOGLOBIN A
WEAK HEMOGLOBIN TEST/CFE
MAXIMUM = 1.27491E-07
MINIMUM = -4.42150E-11
INCREMENT = 3.00000E-08
TIME = 40.000

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 38	ELECTROPHORESIS MODELING CFE TEST RESULTS	DATE: JANUARY 18, 1984



MOLAR CONCENTRATION FOR HEMOGLOBIN A
WEAK HEMOGLOBIN TEST/CFE/WESM/NEG
MAXIMUM = 1.27600E-07
MINIMUM = -1.40366E-11
INCREMENT = 3.00000E-08
TIME = 20.000

ORGANIZATION: USRA/RA1/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 39	ELECTROPHORESIS MODELING CFE TEST RESULTS	DATE: JANUARY 18, 1984



MOLAR CONCENTRATION FOR HEMOGLOBIN A
WEAK HEMOGLOBIN TEST/CFE/WESM/POS
MAXIMUM = 1.27628E-07
MINIMUM = -3.17183E-12
INCREMENT = 3.00000E-08
TIME = 20.000

ORGANIZATION: RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 40	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: FEBRUARY 14,1984

BIER GROUP CASES

M. BIER, O. A. PALUSINSKI, R. A. MOSHER, AND D.A. SAVILLE, March, 1983. ELECTROPHORESIS. MATHEMATICAL MODELING AND COMPUTER SIMULATION. SCIENCE 219, pp. 1281-1287.

THEIR MODEL IS CONSISTENT WITH OURS.
THEY CONFINE ATTENTION TO SINGLE IONIZATION.
THEY COMPUTE FLUXES OF EACH ION SEPARATELY, RATHER THAN AVERAGING OVER THE DEGREES OF IONIZATION AS WE DO.
THEY NEGLECT BULK FLUID MOTION.
THEIR CODE IS LIMITED TO ONE DIMENSION.
THEY ARE PRESENTLY LIMITED TO 5 RADICALS.
THEIR NUMERICAL METHODS ARE MUCH SLOWER AND LESS EFFICIENT THAN OURS.
THEY WERE FIRST!

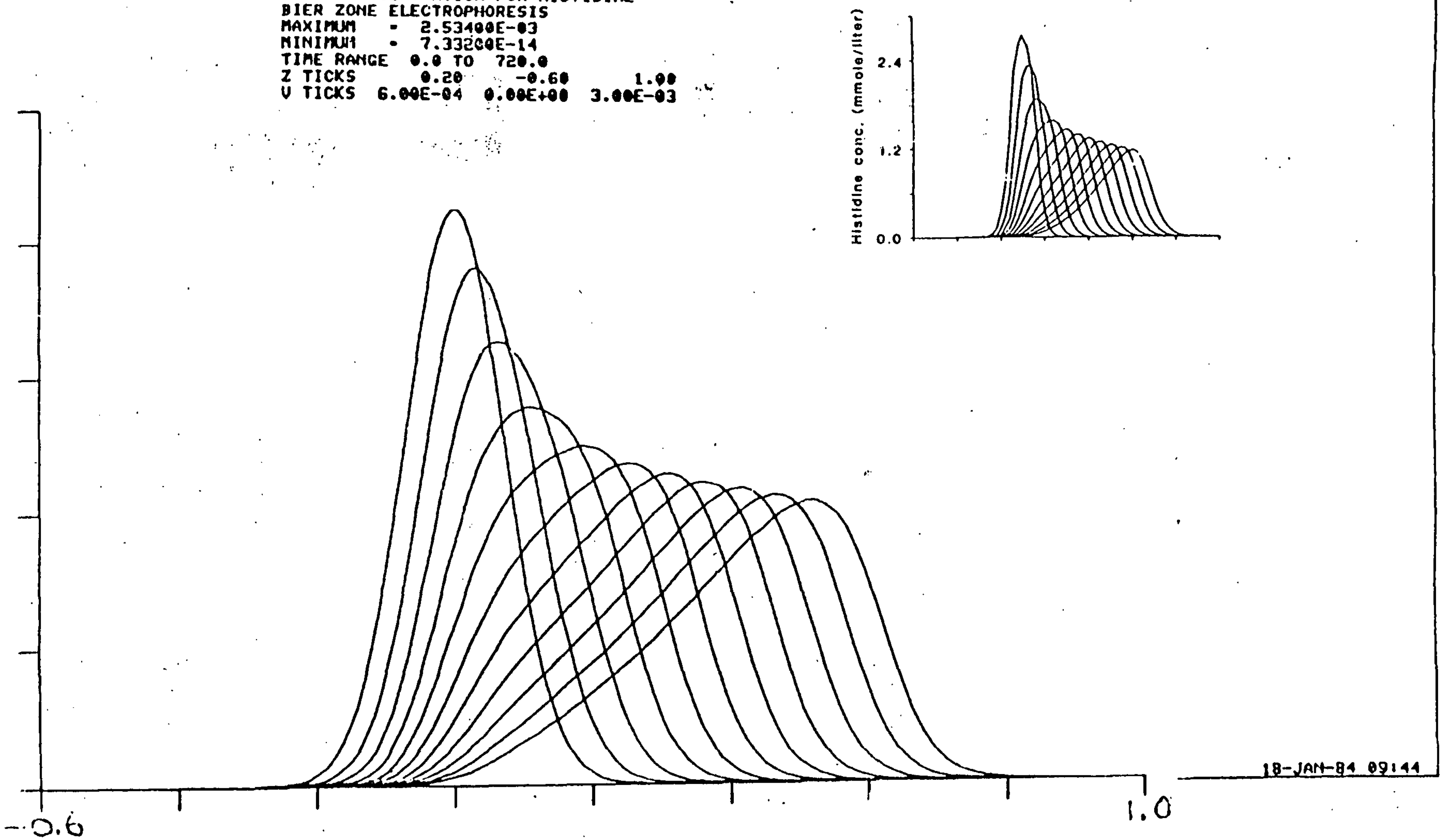
THEY REPORT SEVEN SEPARATE ONE-DIMENSIONAL COMPUTATIONS
- ZONE ELECTROPHORESIS
- MOVING-BOUNDARY (2)
- ISOTACHOPHORESIS (2)
- ISOELECTRIC FOCUSING
- ELECTRODIALYSIS

WE HAVE DUPLICATED ALL SEVEN.

14-FEB-84 07:41

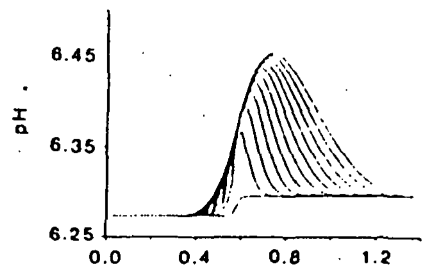
ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 41	ELECTROPHORESIS MODELING BIER VALIDATION RESULTS	DATE: JANUARY 18, 1984

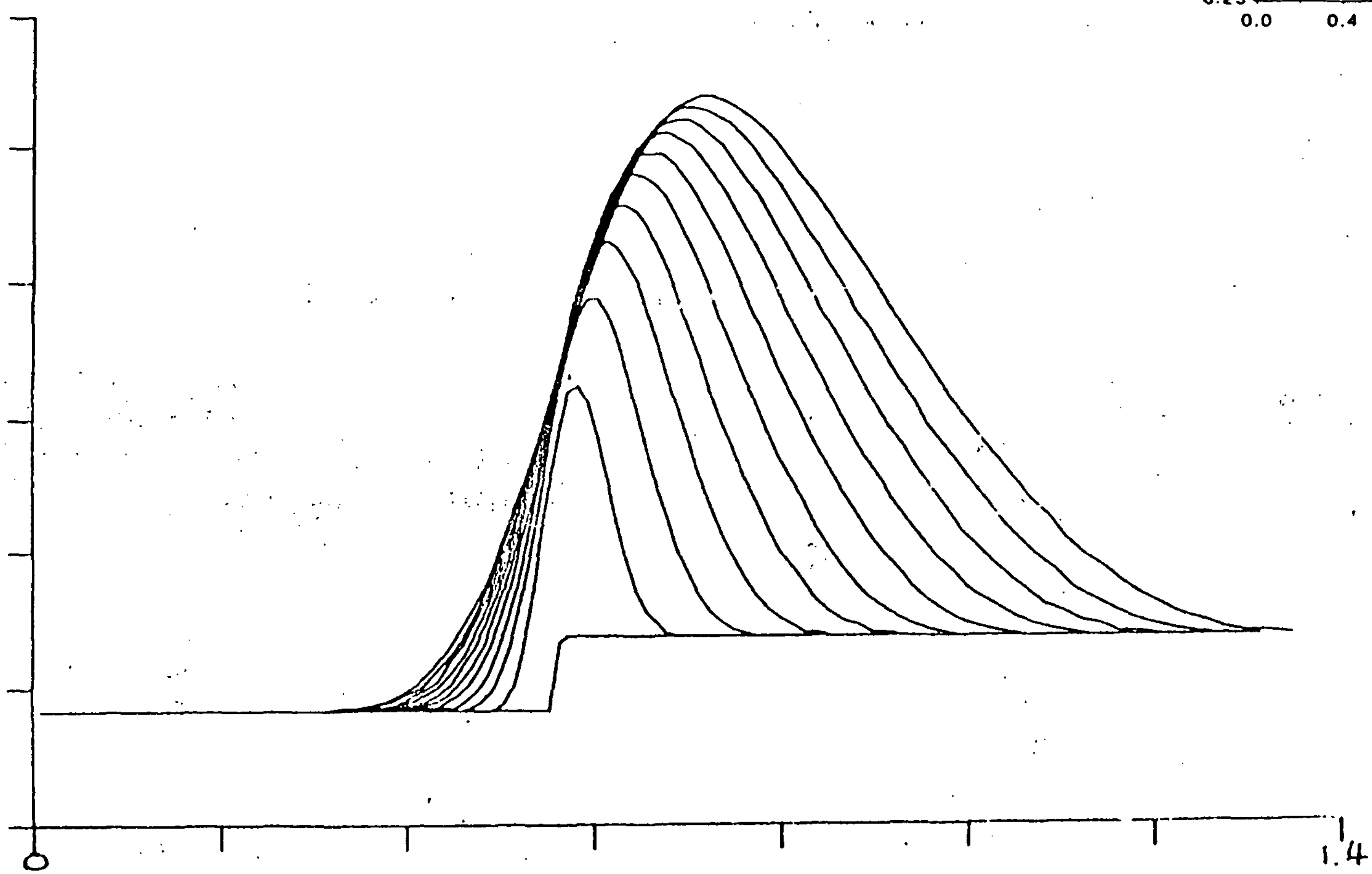
MOLAR CONCENTRATION FOR HISTIDINE
BIER ZONE ELECTROPHORESIS
MAXIMUM = 2.53400E-03
MINIMUM = 7.33200E-14
TIME RANGE 0.0 TO 720.0
Z TICKS 0.20 -0.60 1.00
V TICKS 6.00E-04 0.00E+00 3.00E-03



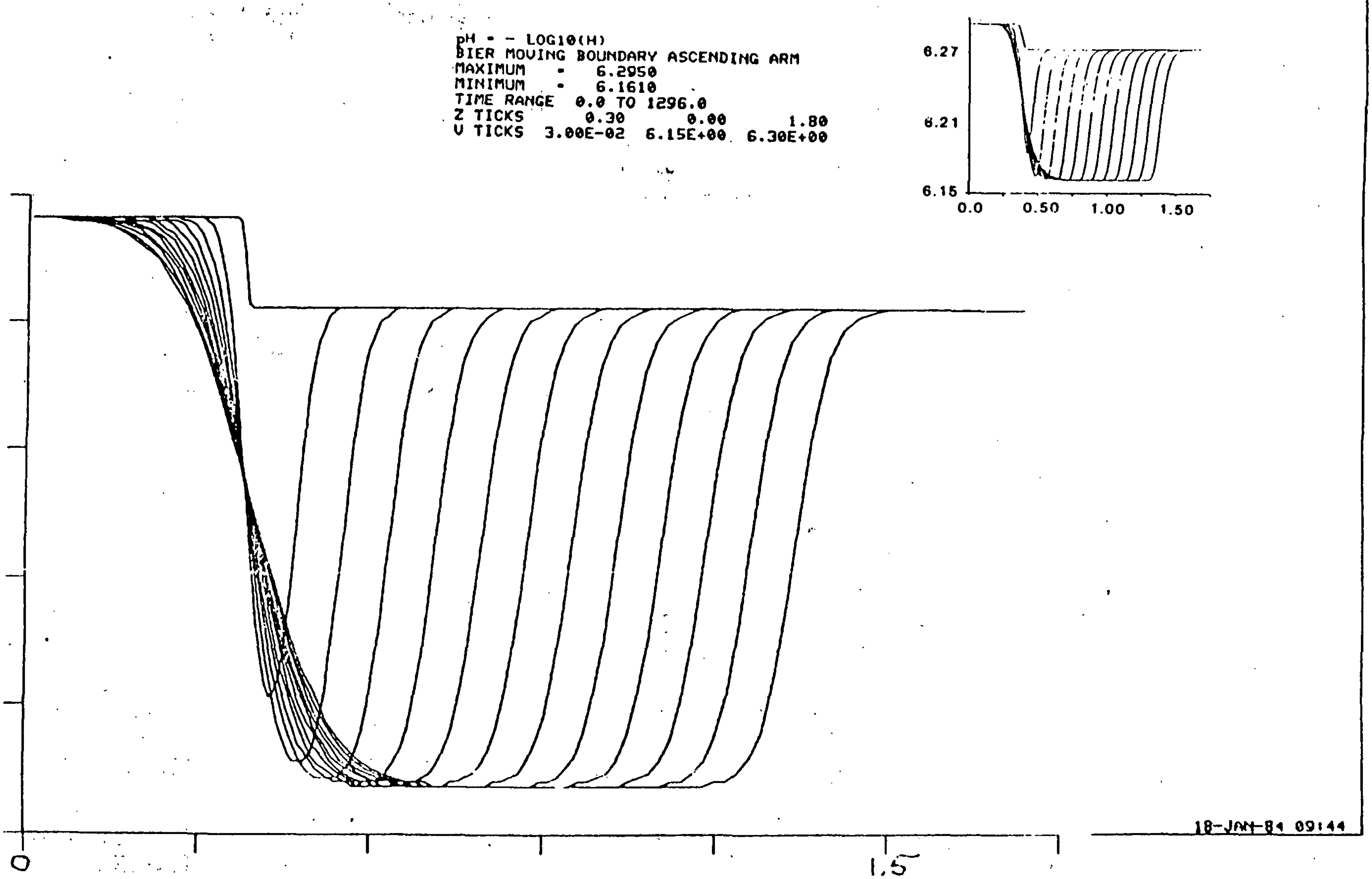
ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 42	ELECTROPHORESIS MODELING BIER VALIDATION RESULTS	DATE: JANUARY 18, 1984

```
pH = - LOG10(H)
BIER MOVING BOUNDARY DESCENDING ARM
MAXIMUM   =    6.4540
MINIMUM   =    6.2730
TIME RANGE   0.0 TO   720.0
Z TICKS       0.20        0.00        1.40
V TICKS   4.00E-02   6.24E+00   6.48E+00
```



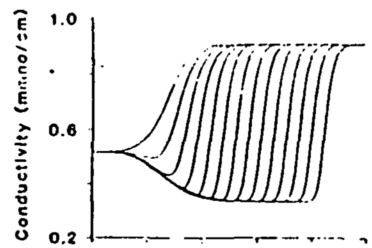


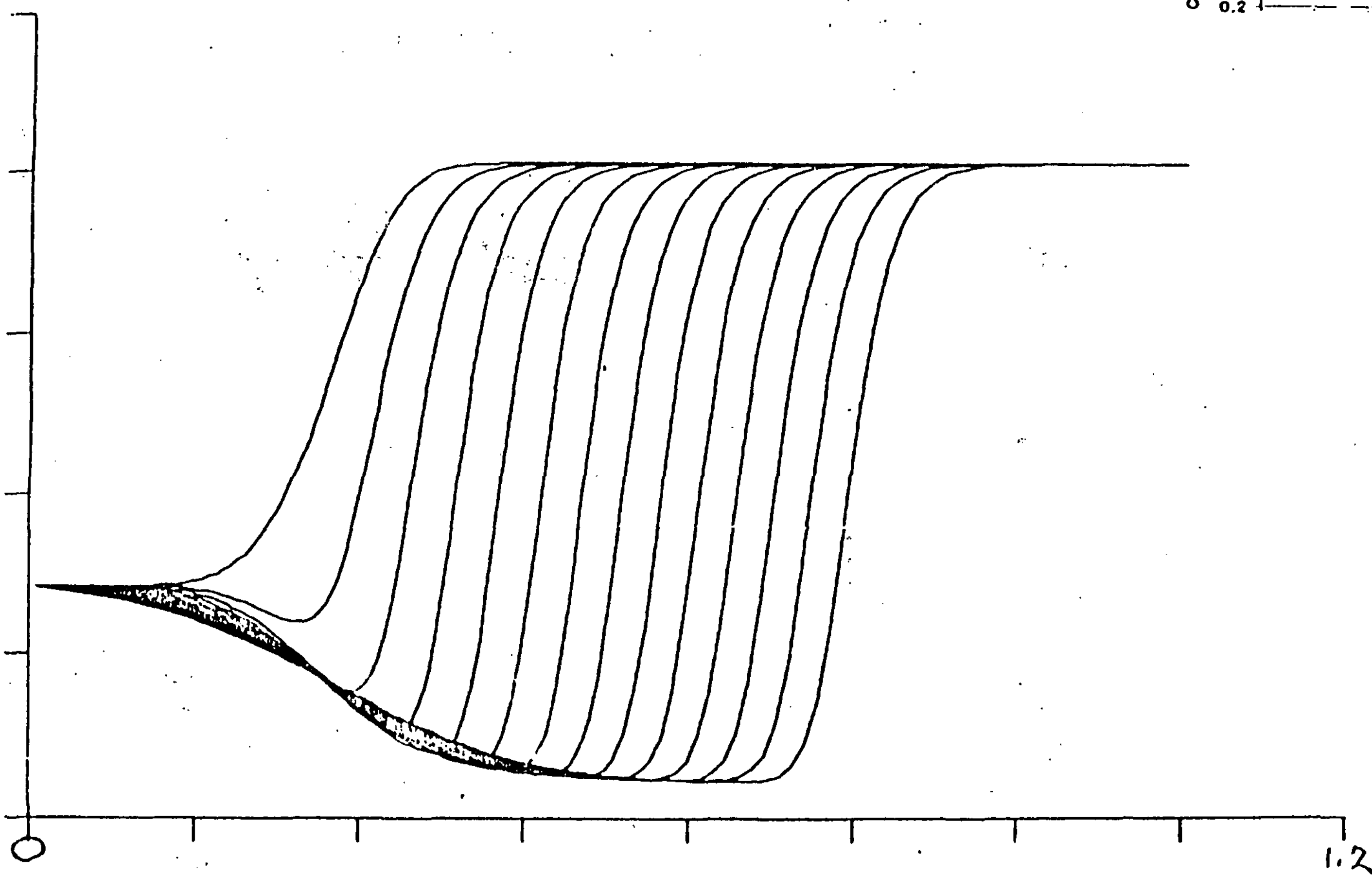
ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 43	ELECTROPHORESIS MODELING BIER VALIDATION RESULTS	DATE: JANUARY 18, 1984



ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 44	ELECTROPHORESIS MODELING BIER VALIDATION RESULTS	DATE: JANUARY 18, 1984

CONDUCTIVITY (MHO/CM)
BIER ISOTACHOPHORESIS, LOW CONCENTRATION
MAXIMUM = 9.06700E-04
MINIMUM = 3.33300E-04
TIME RANGE 0.0 TO 1560.0
Z TICKS 0.15 0.00 1.20
V TICKS 1.50E-04 3.00E-04 1.05E-03





18-JAN-84 09:45

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 45	ELECTROPHORESIS MODELING BIER VALIDATION RESULTS	DATE: JANUARY 18, 1984

```
CONDUCTIVITY (MHO/CM)
BIER ISOTACHOPHORESIS, HIGH CONCENTRATION
MAXIMUM    =  2.20300E-03
MINIMUM    =  5.11200E-04
TIME RANGE  0.0 TO 3120.0
Z TICKS       0.15       0.00       0.90
V TICKS  4.00E-04   4.00E-04   2.40E-03
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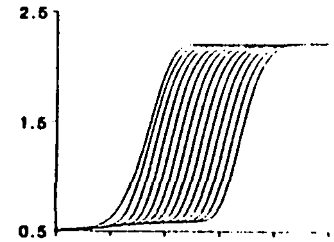
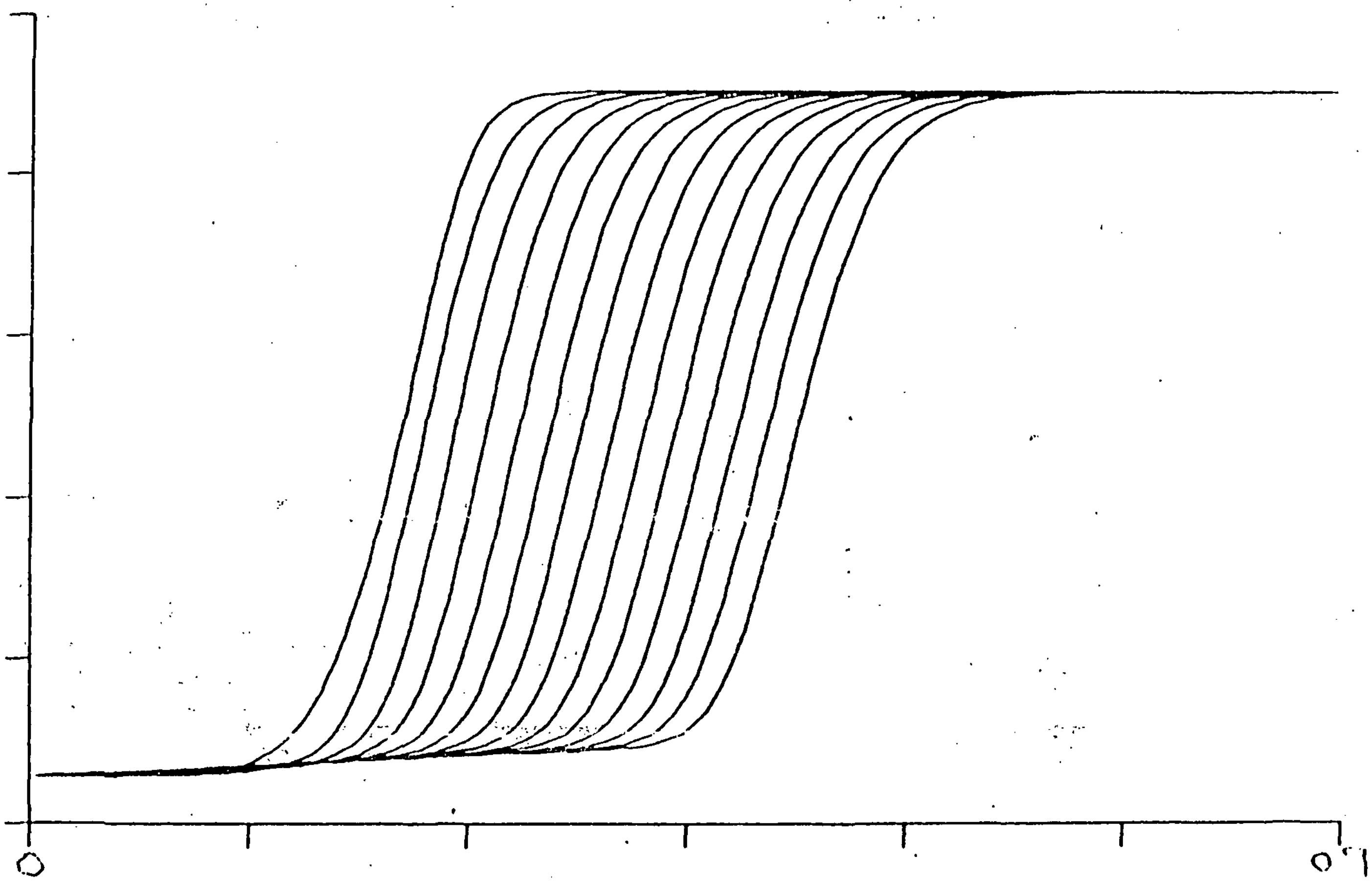
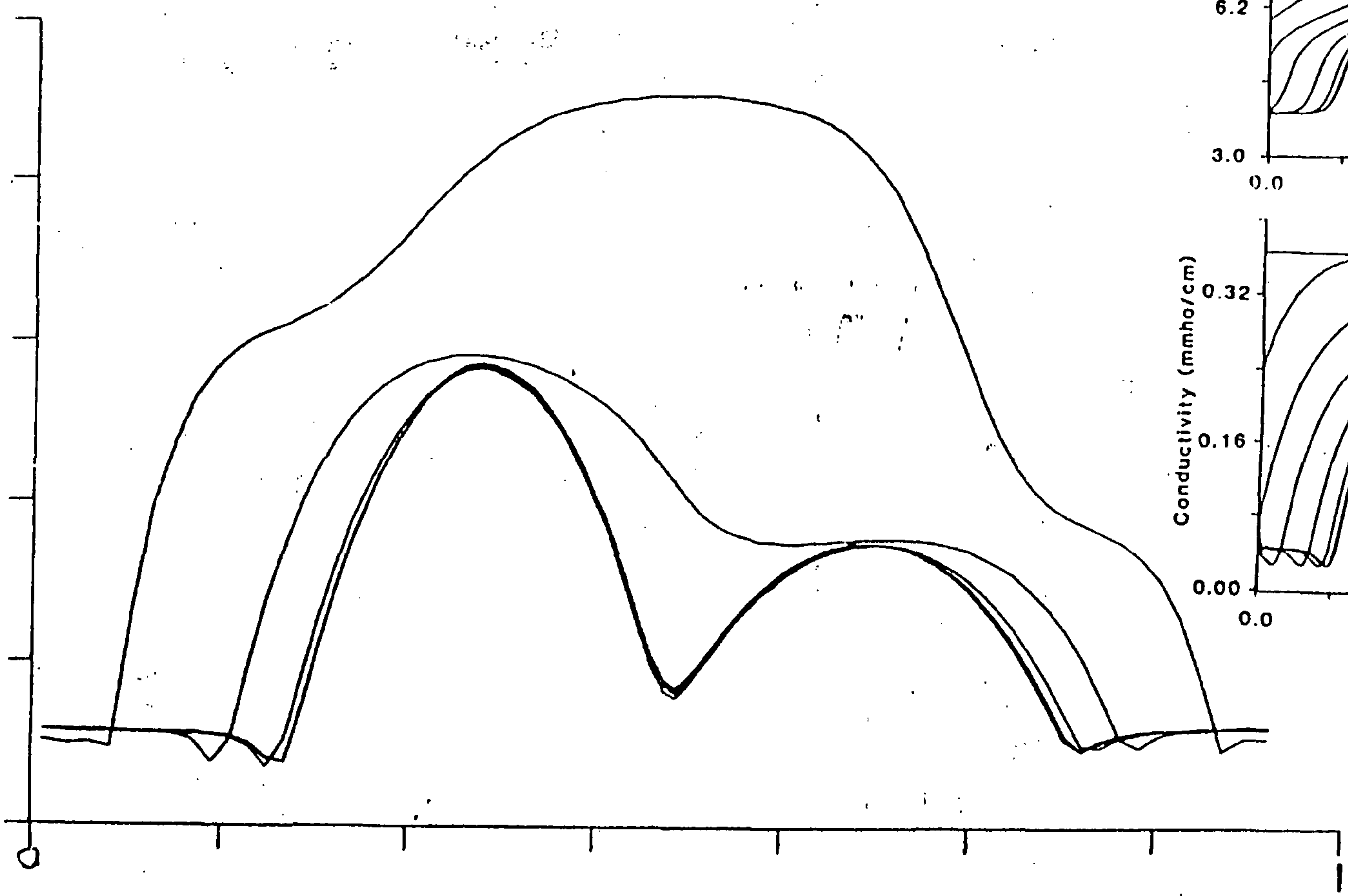


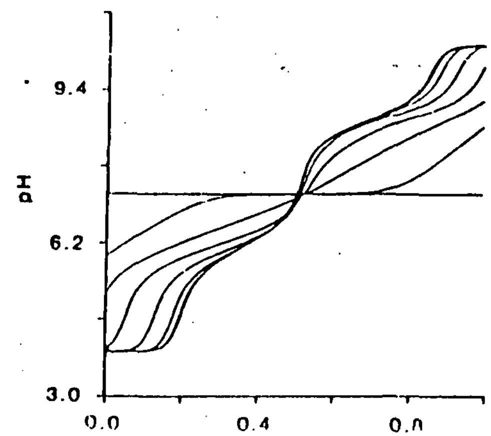


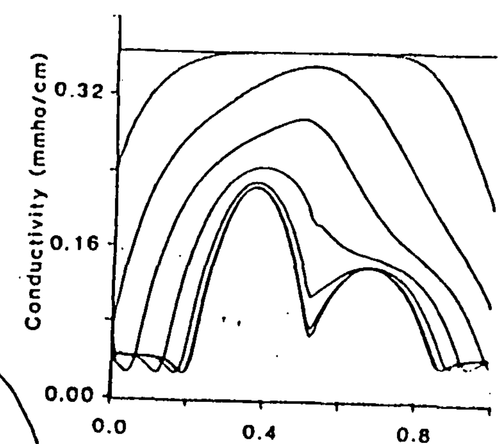
18-JAN-84 09:45

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: RESULTS- 46	ELECTROPHORESIS MODELING BIER VALIDATION RESULTS	DATE: JANUARY 18, 1984

CONDUCTIVITY (MHO/CM)
BIER ISOELECTRIC FOCUSING
MAXIMUM = 3.62100E-04
MINIMUM = 2.88600E-05
TIME RANGE 0.0 TO21600.0
Z TICKS 0.15 0.00 1.05
V TICKS 8.00E-05 0.00E+00 4.00E-04







18-JAN-84 09:45

ORGANIZATION: USRA/RAI/ES73	MARSHALL SPACE FLIGHT CENTER	NAME: GLYN ROBERTS
CHART NO.: PLANS- 47	ELECTROPHORESIS MODELING THE SAMPLE CODE	DATE: JANUARY 18, 1984

PLANS

- SYSTEMATIC TESTS WITH MORE SPECIES
- IMPROVE OUTPUT OPTIONS (MOVIES)
- IMPROVE FORMULATION OF ION MOTION
- INVESTIGATE ANOMALOUS EXPERIMENTAL RESULTS
- RECOMMEND AND INTERACT WITH EXPERIMENTS
- ADD APPROPRIATE DYNAMICS

18-JAN-84 11:39