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MEMORANDUM FOR: Harold Denton, Director
                  Office of Nuclear Reactor Regulation

FROM: Robert B. Minogue, Director
                  Office of Nuclear Regulatory Research

SUBJECT: RESEARCH INFORMATION LETTER 119   DEVELOPMENT OF BEST-
                  ESTIMATE COMPONENT CODE K-FIX (3D, FLX)

I.   INTRODUCTION

    A.   Need for the K-FIX (3D, FLX) Component Code

        There are many two-phase flow processes in reactor components which
        must be analyzed in more detail than can be accomplished by a systems
        code. Such processes include the details of flow near a break in a
        pipe, the behavior of injected ECC water into the downcomer or the
        upper plenum of a PWR, the initial mass and energy flow through a
        break into the containment, the hydraulic forces on the PWR core
        barrel caused by a large break in a pipe, and others. In order to
        study such processes, the Advisory Committee on Reactor Safeguards
        (Ref. 1), the American Physical Society (Ref. 2), and the NRC Office
        of Nuclear Reactor Regulation (Ref. 3) requested the development of
        a calculational tool. The K-FIX (3D, FLX) best-estimate component
        code was developed to meet these requests.

    B.   Evolution of K-FIX (3D, FLX)

        The K-FIX (3D, FLX) Code evolved from the KACHINA Code (Ref. 4).
        The first, two-dimensional version, K-FIX, was issued in 1977 (Ref. 5).
        K-FIX used the implicit multifield calculational technique developed
        for the KACHINA code, but differed from KACHINA in that it implicitly
        coupled phase transition and interfacial heat transfer to the fluid
        dynamics in the iteration calculation for the pressure. The fully
        implicit exchange also led to significant reduction in computation
        time.

        The 2-D version of K-FIX was then extended to 3-D (Ref. 6) to achieve
        the goal of having this two-phase flow dynamics code perform detailed,
        state-of-the-art safety calculations in reactor system components.
        The 3-D capability was especially needed to calculate the asymmetric
        dynamics within the reactor vessel shortly after a cold-leg break.
        This latter problem involves the coupled dynamics between fluid flow
        and structural motion. In order to calculate this fluid-structure
        interaction, the K-FIX (3D) code, which calculated 3-D flows and
        pressure waves within the fluid, was coupled explicitly to the FLX

code (Ref. 7), which solves the three-dimensional elastic-
shell equations in the solid structural material. The
resulting calculational tool is called K-FIX (3D, FLX).
The code was completed and released to the National
Energy Software Center in 1980.

K-FIX (3D, FLX) replaces an earlier code, SOLA-FLX (Ref. 7),
because K-FIX can calculate 3-D effects with a two-fluid
hydrodynamic model, while SOLA-FLX was restricted to 2-D
with a drift-flux hydrodynamic model.

II. DESCRIPTION OF K-FIX (3D, FLX)

A.   K-FIX (3D) (References 5 and 6)

K-FIX (3D) solves the two-fluid conservation equations in three-
dimensional geometry, in either R-θ-Z or X-Y-Z coordinates. Each
fluid phase is described by its own density, velocity, and temperature.
The six field equations for the two phases are coupled through mass,
energy, and momentum exchange. The code is written in a highly
modular form to be easily adaptable to a variety of problems. Thus,
there are separate modules, or subroutines, for each of the inter-
phase exchange terms. These subroutines can be easily changed as
improved models become available.

The viscous stress, viscous work, and the heat conduction terms
within each fluid phase, exist only in the 2-D option; they are
omitted in the 3-D option.

Several boundary conditions are programmed in the code: no-slip
rigid walls; free-slip rigid walls; prescribed inflow; and con-
tinuous outflow. The rigid walls are adiabatic or nonconducting.

The equations are solved using an Eulerian finite difference technique
that implicitly couples the rates of phase transitions, momentum,
and energy exchange to determination of the pressure, density, and
velocity fields. The implicit solution is accomplished iteratively
without linearizing the equations, thus eliminating the need for
numerous derivative forms.

B.   FLX

The FLX code module (Ref. 7) solves the standard three-dimensional
linear-elastic shell equations (Ref. 8) in core barrel geometry.
The top of the core barrel is modeled mathematically as a clamped or
built-in boundary. The bottom of the core barrel is a free boundary
on which forces and moments vanish; only lateral deflections are
considered.

The shell equations are solved numerically by explicitly integrating a system of finite-difference equations. The shell is subdivided into many computational cells that collectively form a two-dimensional computing mesh. The circumferential dimension of each cell is constant, while the axial dimensions can vary from one row of cells to the next. The maximum value of the time-step is limited by inequality conditions obtained from a linear stability analysis.

C.   K-FIX (3D, FLX)

The fluid and structure code modules are coupled together explicitly (Ref. 9). For each calculation cycle, the fluid pressure field is used to determine the differential pressures that drive the shell motion through the radial acceleration equation. The shell equations are often integrated for several time steps per fluid time step, because of their more restrictive stability criteria. After integration through a fluid time step, the shell radial motion is assigned as a boundary conduction to the fluid. The core barrel motion causes a fractional change in volume of the fluid cells adjacent to 'he core barrel, which is responsible for additional terms in the fluid conservation equations.

This coupling technique has been used successfully within one-, two-, and three-dimensional fluid-dynamic simulations. The results with one-dimensional fluid dynamics that exhibit axial, circumferential, and radial motion separately have been compared with analytic effects (Ref. 10).

III.   K-FIX MODEL DEVELOPMENT AND ASSESSMENT

In preparing K-FIX to address blowdown loads, hydrodynamic models were developed and assessed for the most relevant physical processes expected to occur. These included models for: the propagation of pressure waves through a single-phase or two-phase liquid; the nonequilibrium vapor generation that might occur near a break in a pipe; and the critical flow through a break in a pipe, especially for subcooled conditions just upstream of the break.

A.   Shock tube calculations with no phase transitions

Analytical solutions were obtained for wave propagation in a tube separated, by a diaphragm, into two regions initially filled with saturated water-steam mixtures at different pressures (Ref. 11). After the diaphragm is conceptually broken, analytic solutions followed the wave propagation for the case of no-phase transitions between the steam and water. The K-FIX code was applied to this problem and comparison with the exact analytical solution was excellent, as shown in Figure 1 (Ref. 12). Initial phase change models were also used in this study (Ref. 12) as well as in a previous study using the KACHINA Code (Ref. 13). This initial phase change model was soon replaced with a more comprehensive model to be described in the next section.

B. Vapor Generation Model

1. Description of Model (Ref. 14)

The rate of production of vapor mass per unit of the mixture volume is obtained from an equation describing the growth of a given number of bubbles. The rate of growth of the individual bubbles is controlled by conduction of heat within the liquid phase. The liquid thermal diffusivity and the average bubble radius used in this method take into account the combined effects of relative motion between phases and turbulence.

Stated differently, the model considers bubbles, with an initial radius determined by specification of initial values of the void fraction and number of nucleation sites. These bubbles grow at a rate close to but somewhat larger than the conduction controlled rate, because of the enhanced heat transfer from the bulk liquid to the bubble interface due to relative motion and turbulent fluctuations in the liquid. The bubbles continue to grow until they reach a critical size, determined by a Weber number criterion, and then begin to break up. From this point on, the typical bubble size is taken as the critical size and the number of bubbles is determined by the local void fraction.

Both the critical bubble size and the liquid thermal diffusivity depend on the relative velocity between the bubble and the surrounding liquid. The relative velocity is a combination of the difference between the average velocities of liquid and vapor and the contribution due to local turbulent fluctuations in the liquid. To minimize the complexities of the model, in view of the limited departure of the mechanical equilibrium calculations results from data, the model describes the combined effects of these contributing elements by expressing the relative velocity as a product of the liquid velocity and an empirically determined function of void fraction. This empirical function has been tested against critical flow data at both low and high pressures, as described below in Section III.B.2.

2. Comparison with Data

a) Single bubble

A two-dimensional calculation, with several computational cells, was made with K-FIX of the growth of a steam bubble in a 22°K superheated water pool. Comparison with data was good (see Figure 2). A similar calculation of a bubble condensing in a 9°K subcooled water pool was also made, with the evaporation model replaced by a symmetric condensation model. Comparison with data was equally good (Ref.15).

b) Critical Flow

i. Various nozzles at high pressure (Ref. 14)

A comparison of K-FIX calculations was made with
critical flow data from two Semiscale tests and two
Marviken tests. For each test, two calculations were
made, one with the nonequilibrium vapor generation
model described in the previous section and one with
a very large vapor generation rate that produces,
very nearly, continuous equilibrium states in which
the liquid, saturation, and vapor temperatures are
the same. The two Semiscale tests were S-02-4 with a
Henry nozzle, and S-06-5 with a LOFT counterpart
nozzle. The comparison of the measured and calcu-
lated flow rates for test S-06-5 are shown in Figure 3.
Substantial nonequilibrium exists at an early time
for these tests when subcooled water enters the
nozzle and the nonequilibrium model agrees much
better with the data than does the equilibrium model;
the latter underpredicts the flow rate. Two-phase
flow enters the nozzle at later times during which
both equilibrium and nonequilibrium models give
reasonable agreement with the data.

To investigate the predictive capability of the model
at large scale, calculations were performed for two
blowdown tests of a series made at the Marviken test
facility. Test 1 featured a nozzle throat diameter
17 times larger than in the Semiscale tests while the
nozzle used in Test 4 was 29 times larger. The
comparison of K-FIX calculations with measured flow
rates for Test 1 is shown in Figure 4. Subcooled
water enters the nozzle for about 60 seconds. The
nonequilibrium model gives a much better simulation
of the data than does the equilibrium model.

ii. Various nozzles at low pressure (Ref. 16)

As a further check of the nonequilibrium vapor genera-
tion model, low pressure data from the MOBY DICK and
BNL test facilities were analyzed. These tests
involved fluid pressures between 0.1 and 0.4 mPa and
temperatures around 373°K.

Extension of the nonequilibrium model to those low
pressures was achieved by expanding the functional
relationships for the turbulence intensity and the
nucleation sites per unit volume to the lower pres-
sure range. The calculational results obtained at

higher pressures remain unchanged. Inlet pipe
diameters to the test sections are 2 and 5 cm, for the
MOBY DICK and BNL experiments, respectively. Detailed
axial profiles of pressure and void fraction were
measured in both facilities. A comparison of K-FIX
results with measured axial pressure profile in MOBY
DICK is shown in Figure 5. Similar good agreement was
also obtained with the BNL data.

IV. FLX MODEL DEVELOPMENT AND ASSESSMENT

A description of the standard three-dimensional, linear-elastic
shell equations solved by the FLX code is given in Reference 7.
The FLX code has been checked by comparisons with a variety of
analytic solutions (Refs. 17, 18, and 19). The comparisons include
calculations of added mass effects, core barrel torsional vibration
modes and frequencies, lateral vibration frequencies that include
effects of both shear and bending, and breathing mode vibrations.
Limited comparisons with small-scale test data have also been made
(Ref. 20).

Two examples of comparison of FLX results with exact analytic solutions
for core barrel geometry are given in Figures 6 and 7. The deflection
profiles for the fundamental mode associated with the Timoshenko and
classical beam equations' solutions and the FLX solution are compared in
Figure 6. The FLX solution and the solution to the Timoshenko's equations
are in quite good agreement.

The HDR test facility in Germany is investigating the loads on a core
barrel, with an added mass ring on the bottom, during the initial stage
of a cold-leg blowdown (Refs. 18 and 25).

The frequency and mode shape of HDR core barrel motion initiated by
torsion about the longitudinal axis has also been determined analytically
including the mass ring. The FLX calculation exhibits a torsional fre-
quency of 22.0 Hz which agrees precisely with the analytic solution. The
mode shapes are compared in Figure 7 at the end of one period and are
also in excellent agreement.

V.   K-FIX APPLICATIONS

A.   Multidimensional Effects in Critical Flow (Ref. 21)

Flow multipliers are typically used to make one-dimensional critical
flow calculations agree with data. Two-dimensional calculations
were performed with K-FIX and compared with 1-D calculations, both
without the use of any artificial flow multipliers or break models
to see if multidimensional velocity distributions in the nozzle
could explain the need for break flow mutipliers. The 2-D calcula-
tions gave good agreement with flow data while the 1-D calculations
were typically higher than the data (Ref. 21). The calculated break

flow multipliers needed to bring 1-D calculations in agreement with
2-D calculations for various length to diameter nozzle ratios are
shown in Figure 8. The break flow multiplier curve does not represent
a universal function for nozzles. In particular, it does not extend
into very small L/D ratios typical of orifices. Nevertheless,
calculations on a variety of practical entrance and exit geometries
have shown that the corrective discharge multiplier shown in Figure 8
is correct to within a few percent.

B.   PRETEST PREDICTIONS FOR HDR BLOWDOWN TESTS USING K-FIX (3D, FLX)

Under an agreement with the Federal Republic of Germany, the USNRC
is supplying pretest prediction for selected blowdown load tests
run on the HDR facility. Prior to performing these pretest pre-
dictions, a series of check-out and sensitivity calculations were
run on HDR geometry with the K-FIX (3D, FLX) Code (Refs. 18 and 22).
Pretest prediction results were submitted to both the USNRC (Ref. 23)
and the HDR project (Ref. 24). The results of the two calculations
were almost identical, but the one submitted to the NRC included the
effect of two large pipes connected to the vessel.

The sample comparisons of these pretest prediction results with
data measured in HDR Test V 31.1 are shown in Figures 9 and 10 for the
pressure difference across the core barrel and for the local core
barrel displacement, respectively (Ref. 25). The agreement of K-FIX
(3D, FLX) results with the data for this test was excellent.

C.   DISTRIBUTION OF WATER INJECTED INTO A PWR UPPER PLENUM

As part of the USNRC commitment to provide calculations for the
2D/3D International Refill/Reflood Program, K-FIX was used to calculate
the multi-D distribution of water injected from a hot leg into the
upper plenum of a German design PWR (Ref. 26). Calculations were
first compared with proprietary KWU data on water injected into a
full-size PWR upper plenum filled with air at room temperature and
pressure. Considering the uncertainties in the data, the agreement
of K-FIX was quite adequate. The calculations were then repeated,
this time considering the effects of steam condensation on the
injected water. Comparison of the air-water and steam-water calcula-
tions gave a first indication of the potential effectiveness of
hot-leg ECC injection.

VI   USE OF K-FIX FOR NRC SAFETY CONCERNS

K-FIX (3D, FLX) is a valuable calculational tool for addressing the
Generic Issue A-2, effect of asymmetric blowdown loads on vessel supports
and vessel internals. This code, along with HDR test results, can also be
used for auditing and assessing vendor calculations of blowdown loads.

K-FLX (3D, FLX) can be used either with or without fluid-structure
coupling to assess the vendor codes that either do or do not include
this effect.

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Robert B. Minogue, Director
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Enclosures: Figures 1
  through 10

cc w/encls:
R. Mattson, NRR
P. Check, NRR
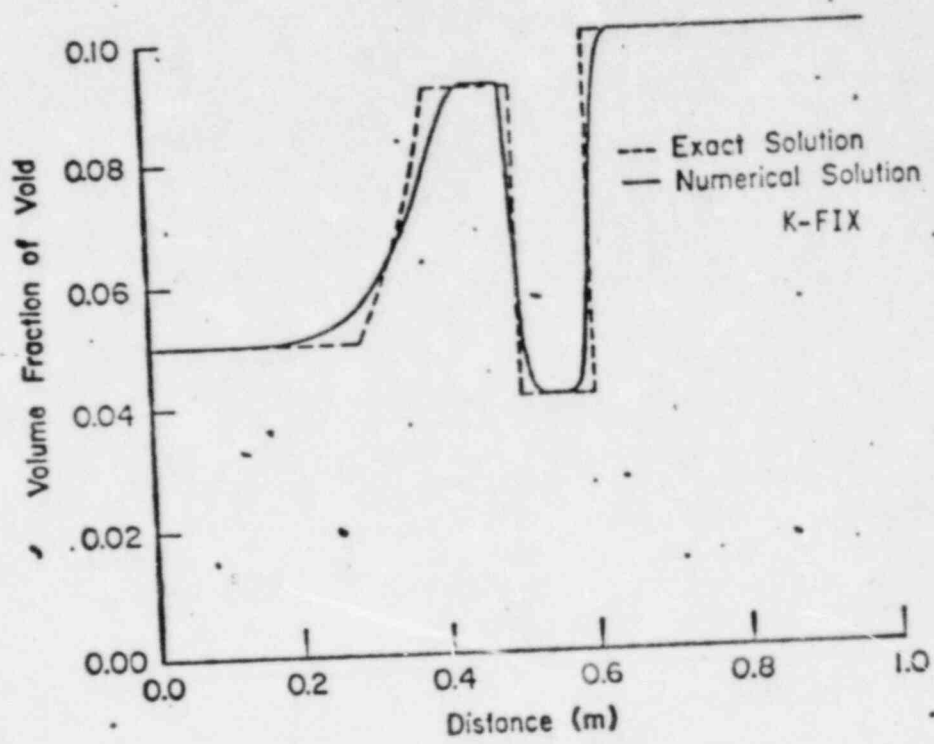T. P. Speis, NRR
E. Throm, NRR
G. W. Knighton, NRR

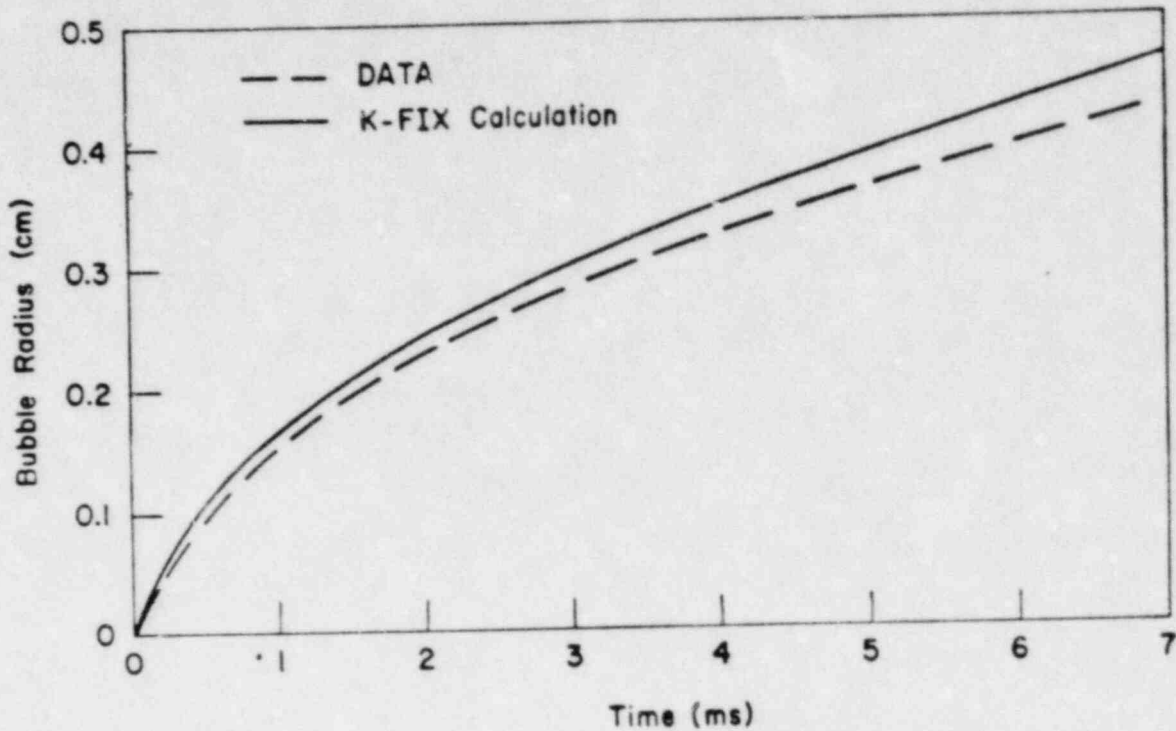FIG. 1 | Volume fraction of void profiles at t = 2 ms without phase change.

FIG. 2   Radius of an isolated steam bubble growing in a superheated water pool.
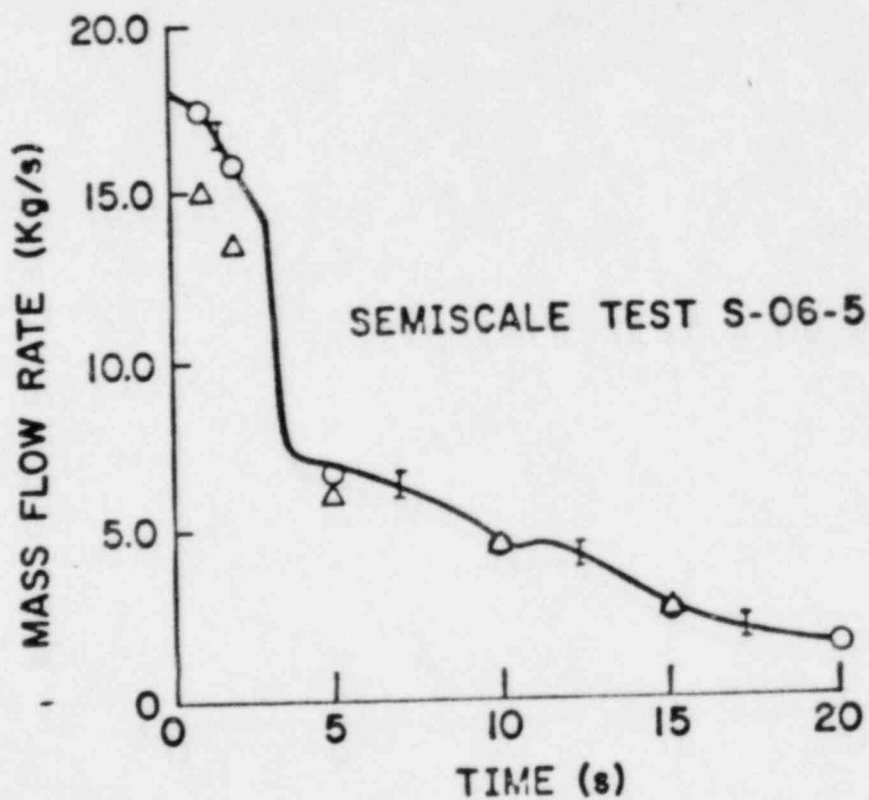
FIG. 3   Comparison of the measured mass flow rate (—) from Ref. 20, the computed mass flow rate with the nonequilibrium model (o), and the computed mass flow rate for equilibrium (△).
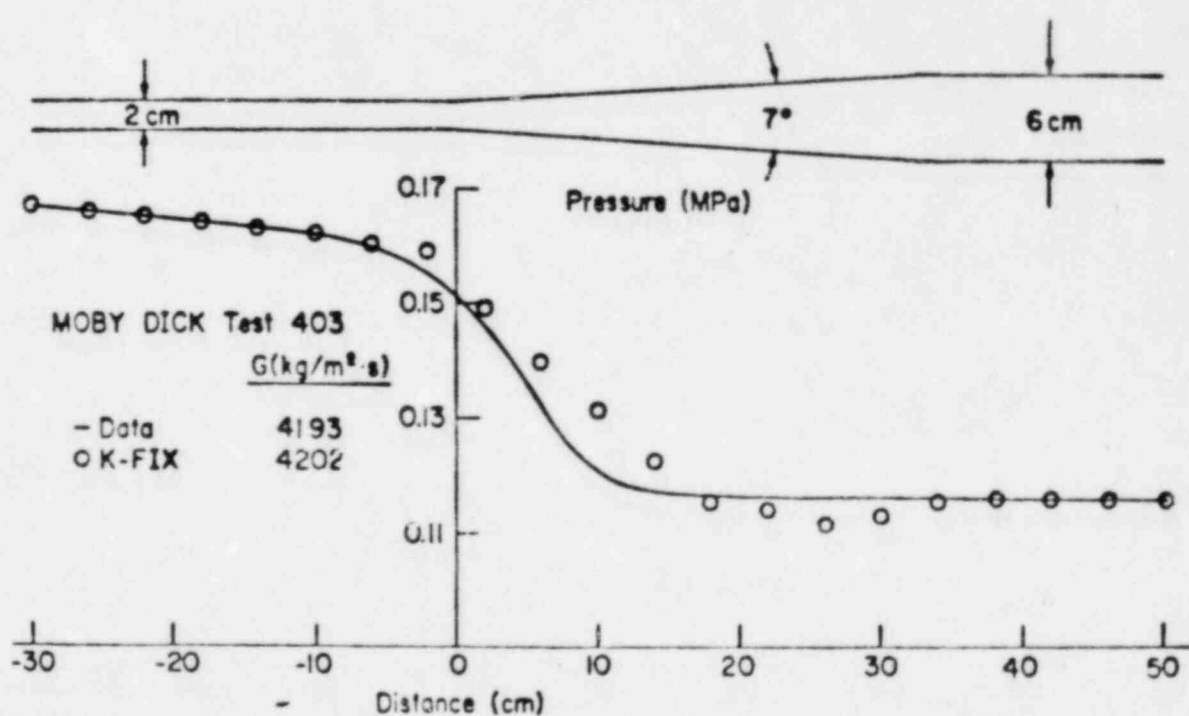
MARVIKEN TEST I
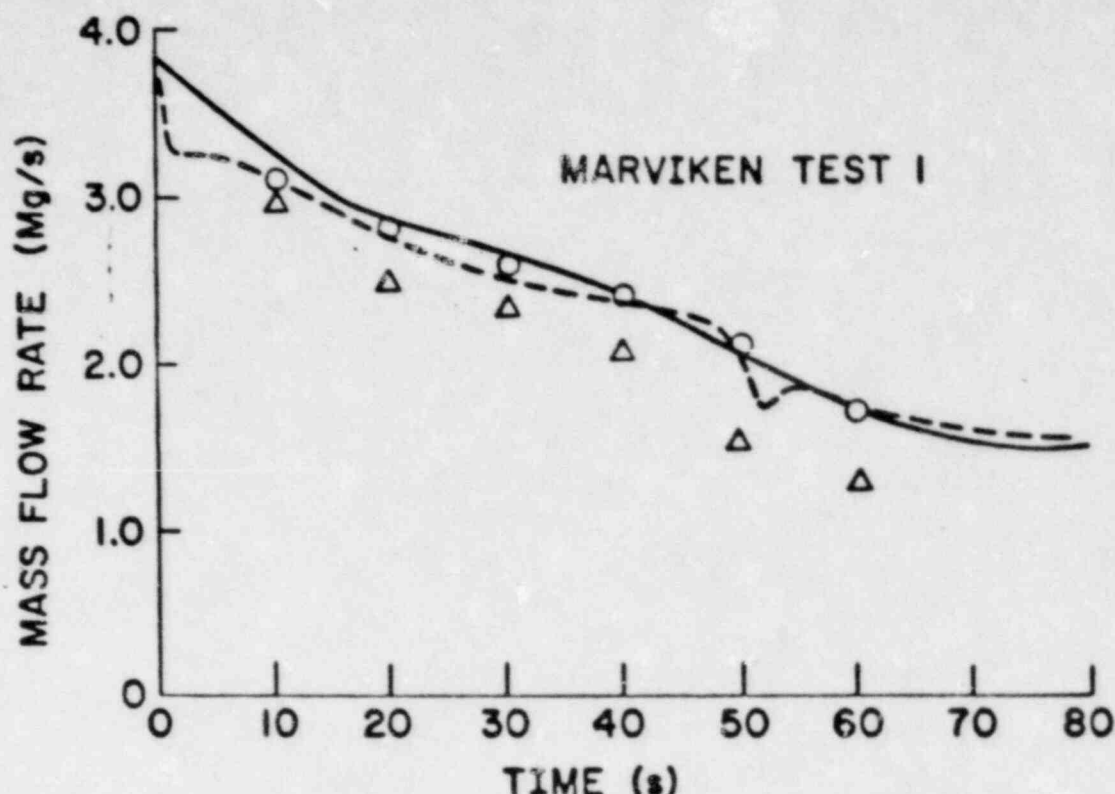
FIG. 4 Comparison of the measured mass flow rate determined by vessel mass change (—) and pitot-static velocity profile (---), the computed mass flow rate with the non-equilibrium model (o), and the computed mass flow rate for equilibrium (Δ).

MOBY DICK Test 403

	G(kg/m²·s)
– Data	4193
O K-FIX	4202

FIG. 5 MOBY DICK nozzle geometry and measured axial pressure profile for test 403. The calculated values were obtained for non-equilibrium (0) vapor production.
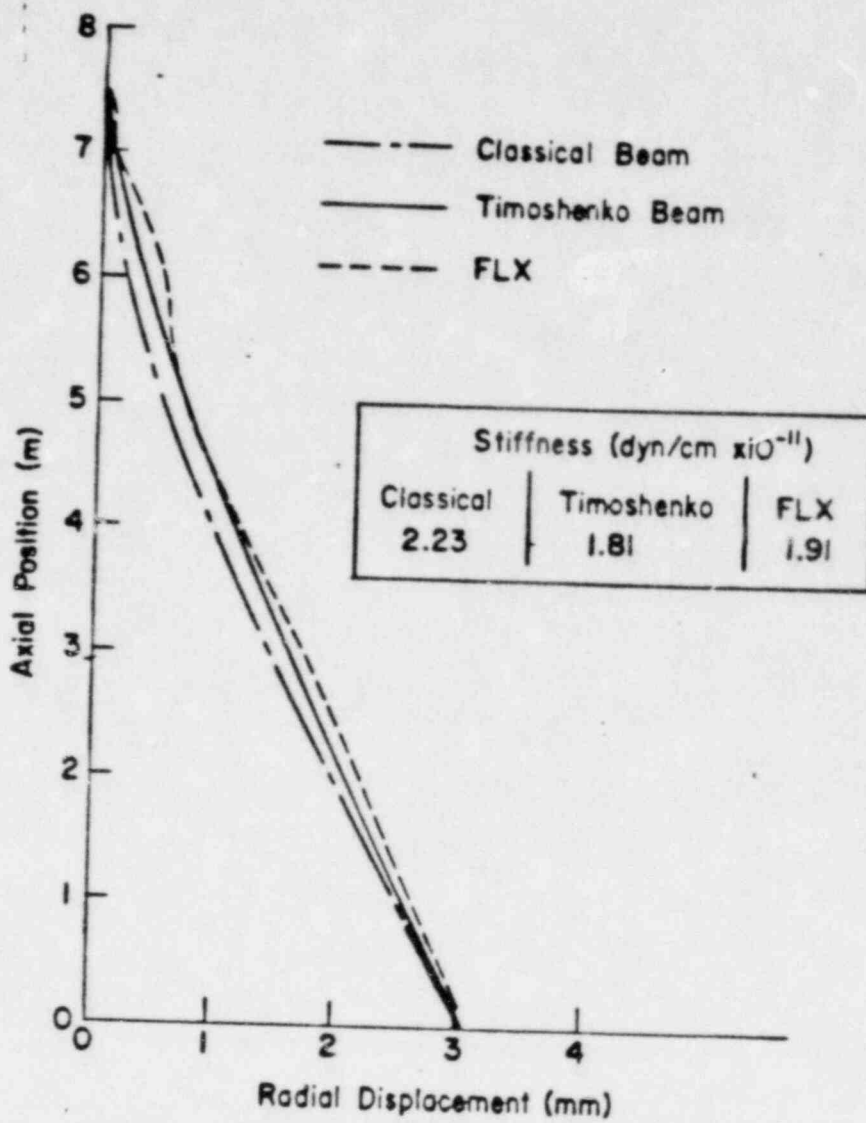
FIG. 6   Fundamental mode shape calculated with FLX compared with analytic results for solutions of the classical and Timoshenko beam equations.
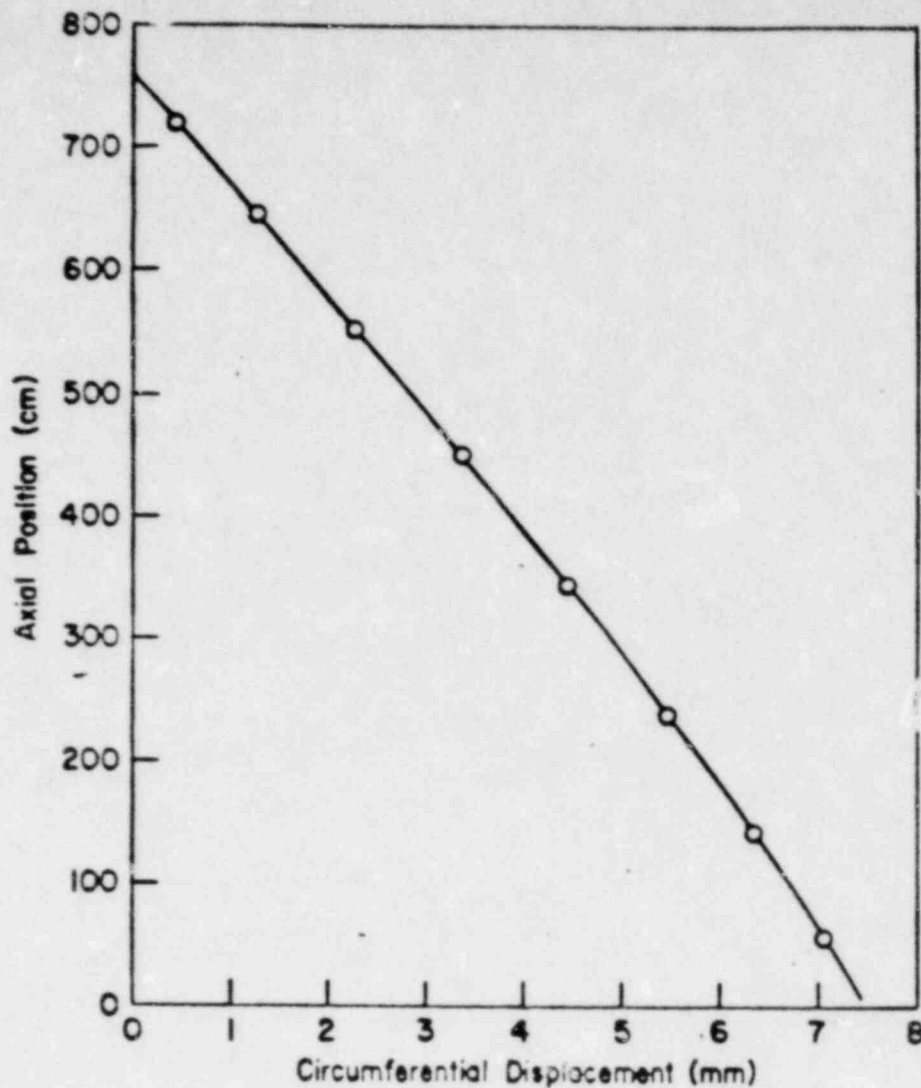
FIG. 7   Fundamental torsional mode shape calculated with FLX compared
with the analytic result. The calculated torsional frequency is
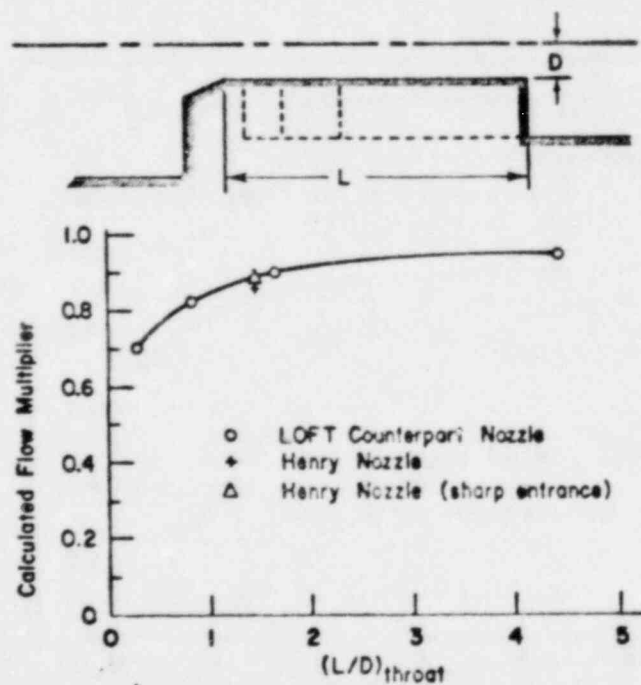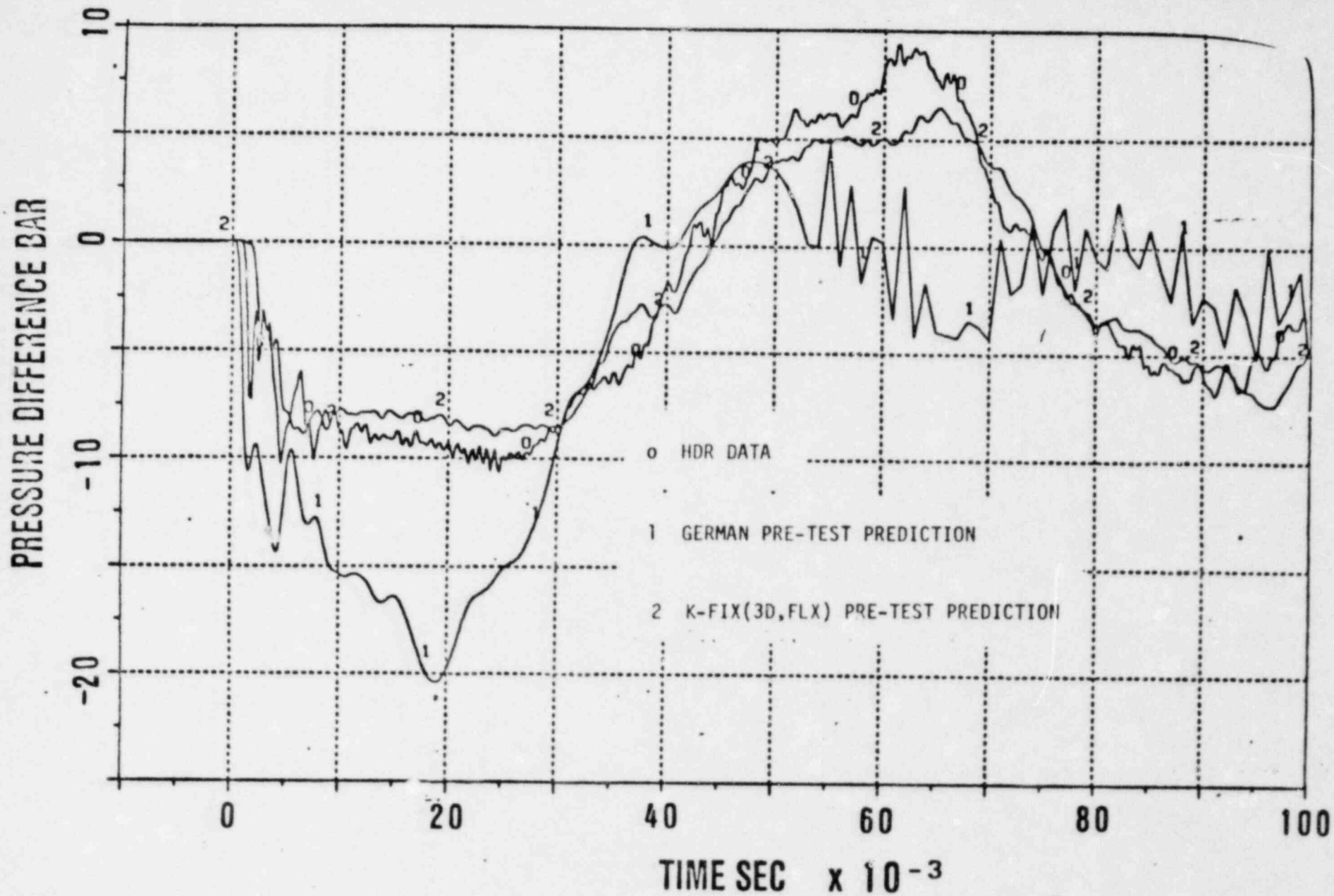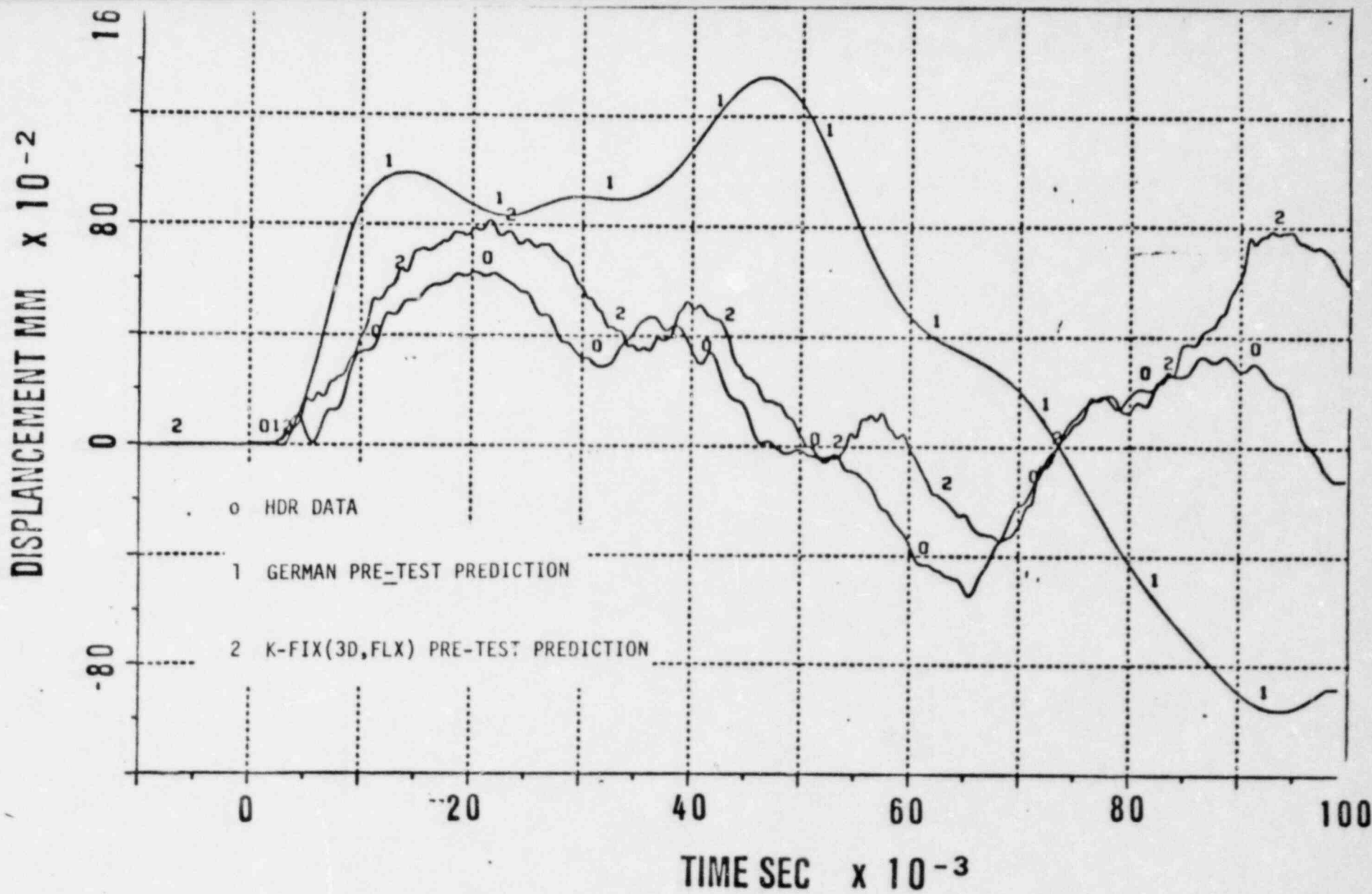22.0 Hz, which agrees precisely with the analytic solution.

FIG. 8   Effect of throat length to throat diameter ratio

Comparison Between Experiment and Predictions for the Pressure Difference (V31.1)

FIG. 9

Comparison Between Experiment and Predictions for the
Displacement   (V31.1)

FIG. 10

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