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FORCE2: A STATE-OF-THE-ART TWO-PHASE CODE FOR HYDRODYNAMIC CALCULATIONS*

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ABSTRACT

A three-dimensional computer code for two-phase flow named FORCE2 has been developed by Babcock and Wilcox (B & W) in close collaboration with Argonne National Laboratory (ANL). FORCE2 is capable of both transient as well as steady-state simulations. This Cartesian coordinates computer program is a finite control volume, industrial grade and quality embodiment of the pilot-scale FLUFIX/MOD2 code and contains features such as three-dimensional blockages, volume and surface porosities to account for various obstructions in the flow field, and distributed resistance modeling to account for pressure drops caused by baffles, distributor plates and large tube banks. Recently computed results demonstrated the significance of and necessity for three-dimensional models of hydrodynamics and erosion.

This paper describes the process whereby ANL's pilot-scale FLUFIX/MOD2 models and numerics were implemented into FORCE2. A description of the quality control to assess the accuracy of the new code and the validation using some of the measured data from Illinois Institute of Technology (IIT) and the University of Illinois at Urbana-Champaign (UIUC) are given. It is envisioned that one day, FORCE2 with additional modules such as radiation heat transfer, combustion kinetics and multi-solids together with user-friendly pre- and post-processor software and tailored for massively parallel multiprocessor shared memory computational platforms will be used by industry and researchers to assist in reducing and/or eliminating the environmental and economic barriers which limit full consideration of coal, shale and biomass as energy sources, to retain energy security, and to remediate waste and ecological problems.

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NOMENCLATURE

a,b	Transport coefficients (see Eq. 15)
C_d	Drag coefficient (see Eq. 8)
c	Compaction modulus
d_p	Particle diameter, m
g	Acceleration due to gravity in the x, y, and z-directions, = g_x, g_y, g_z, m/s^2
G_k	Solids elastic modulus for phase k ($G_f = 0$), Pa
$\bar{\bar{I}}$	Unity tensor
L	Characteristic length or mean free path, m
$\overline{M}$	Molecular weight, kg/mol
$\dot{m}_k$	Mass source for phase k, $kg/(m^3 \cdot s)$
p	Pressure, Pa
$\overline{R}$	Universal gas constant in the ideal gas law, J/(mol·K)
R_i	Flow resistance coefficients for flow in the x-, y-, and z-directions, = R_x, R_y, R_z, m^{-1}
Re	Reynolds Number
S	Source term
v_k	Velocity of phase k, m/s

Greek Letters

β_A, β_B	Fluid-particle friction (drag) coefficients for hydrodynamic models A and B, respectively, $kg/(m^3 \cdot s)$
γ_v	Volume porosity

γ_l	Surface permeabilities in the x-, y-, and z-directions, $= \gamma_x, \gamma_y, \gamma_z$
ε_k	Volume fraction of phase k, $\varepsilon_f = 1 - \varepsilon_s$, $\varepsilon_f = \varepsilon$
ε^*	Compaction gas volume fraction
ζ_k	A parameter used to select the hydrodynamic model for phase k
κ_k	Bulk viscosity of phase k, Pa·s
μ_k	Microscopic viscosity of phase k, Pa·s
ρ_k	Microscopic density of phase k, kg/m^3
ρ'_k	Macroscopic density of phase k, $= \varepsilon_k \rho_k$,
$\bar{\bar{\tau}}_k$	Viscous stress of phase k, Pa
ϕ	Dependent solution variable (see Eq. 15) or sphericity (also called shape factor) of solids
ψ	Dependent solution variable (see Eq. 15)

Subscripts

A	Hydrodynamic model A
B	Control volume in back of volume P or hydrodynamic model B
E	Control volume east of volume P
F	Control volume in front of volume P
N	Control volume north of volume P
P	Control volume of interest
Q	Subscript used to denote quantities at the center of main control volumes (see Eq. 15)
S	Control volume south of volume P
W	Control volume west of volume P
b	Back face
e	East face
f	Fluid phase or front face
i,k	Phase i or k (i = f,g, k = f,g)
p	Particle
q	Subscript used to denote quantities on the faces of a main or momentum control volume (see Eq. 15)
s	Solids phase or south face
w	west face

Operators

$\nabla \cdot$	Divergence
∇	Gradient

1. INTRODUCTION

Solids motion (and the associated bed dynamics involving bubble evolution and pressure fluctuations) is the key to understanding the erosion processes in fluidized-bed combustors (FBCs). Fluidized-bed combustors used industrially continue to show promise for burning high sulfur coal, but erosion of in-bed tubes and other components is still hampering the commercialization of the FBC technology. Despite its importance, the exact mechanisms of erosion and hydrodynamics in fluidized beds are poorly understood. Many models have been proposed for studying hydrodynamic phenomena in fluidized-bed combustors. Most of them are one- or two-dimensional models. The one-dimensional models, which include chemical reaction and pollutant formulation rely heavily on simplifying assumptions.

Recently, three-dimensional models for gas-solids flow have been developed with a constant microscopic solids viscosity at IIT (Illinois Institute of Technology) (Gidaspow and Ding, 1990) and at B & W (Babcock & Wilcox) (Burge, 1991) and with a kinetic theory model for hydrodynamics and erosion at ANL (Argonne National Laboratory) (Ding and Lyczkowski, 1992). Application of these models to studying gas-solids fluidization phenomena has been successfully carried out. Comparisons between computed results and experimental data have shown the significance of and necessity for three-dimensional models of hydrodynamics and erosion in bubbling fluidized beds (Ding and Lyczkowski, 1992). To date, no other published three-dimensional two-phase flow models have been used to simulate fluidized beds, to our knowledge. One reason is the extensive computing cost.

In this paper, the FORCE2 three-dimensional models for two-phase flow are briefly described and validation is demonstrated with modeling of gas-solids fluidized beds. Since the fluidized bed is inherently oscillating with no true steady-state ever achieved, our hydrodynamic computer modeling is time-dependent.

2. HYDRODYNAMIC MODELS

The hydrodynamic approach to fluidization which was started by Davidson (1961) is the basis for the models implemented in FORCE2. All the solid particles having identical densities and diameters form a continuum. The fluid and solids phases are then treated as interpenetrating fluids in an Eulerian formulation. Conservation of mass and momentum are then applied to each phase (a total of two or more) to derive the hydrodynamic model. Both single and multiple particle phases have been simulated with this approach (Gidaspow, 1986). The current FORCE2 model considers only two phases: one fluid phase, which can be a gas or liquid and one solids phase. The capabilities of several computer codes utilizing this approach were reviewed by Smoot (1984) and Gidaspow (1986). Work at ANL using the FLUFIX/MOD2 computer code (Lyczkowski and Bouillard, 1992) to model IIT's small-scale thin "two-dimensional" fluidized bed has provided partial validation of the hydrodynamic model.

Two hydrodynamic models, called Models A and B by Lyczkowski and Bouillard (1992) have been implemented in FORCE2. They are extensions of the models developed by Lyczkowski et al. (1990, 1992) for the FLUFIX code. The models have been extended in FORCE2 to include: (1) three-dimensional Cartesian geometry; (2) volume porosities and surface permeabilities to account for volume and surface obstructions in the flow field, and (3) distributed resistance to account for pressure drops caused by baffles, distributor plates, and large tube bundles. The hydrodynamic models of fluidization uses the principles of conservation of mass, momentum, and energy. The continuity equations and the separated phase momentum equations for three-dimensional,

transient, and isothermal two-phase flow in Cartesian coordinates are given below.

Continuity equations

$$\frac{\partial}{\partial t}(\rho'_k\gamma_v) + \nabla\cdot(\rho'_k\gamma_i v_k) = \gamma_v\dot{m}_k \tag{1}$$

where $\rho'_k = \varepsilon_k\rho_k$ is the macroscopic density, the subscript k denotes the phase (i.e., k = f for the fluid phase and k = s for the solids phase), ε_k is the phase volume fraction, γ_i are the surface permeabilities, γ_v is the volume porosity, and v_k is the phase velocity vector.

Momentum equations

$$\frac{\partial}{\partial t}(\rho'_k\gamma_v v_k) + \nabla\cdot(\rho'_k\gamma_i v_k v_k) = -\zeta_k\gamma_v\varepsilon_k\nabla p + \gamma_v\rho'_k g - \gamma_v R_i\frac{\rho'_k v_k^2}{2} - \gamma_v\beta_M(v_i - v_k) + \gamma_v G_k\nabla\varepsilon_g + \nabla\cdot\bar{\bar{\tau}}_k \tag{2}$$

where

$$\bar{\bar{\tau}}_k = \varepsilon_k\mu_k\gamma_i\left[\nabla v_k + (\nabla v_k^T)\right] - \gamma_i\varepsilon_k\lambda_k(\nabla\cdot v_k)\bar{\bar{I}}, \tag{3}$$

and

$$\lambda_k = \frac{2}{3}\mu_k - \kappa_k \tag{4}$$

κ_k is the bulk viscosity for phase k. The parameter, ζ_k, is used to select the hydrodynamic model according to model A or model B. For model A, $\zeta_{f,s} = 1$ for both the fluid and the solids phase. For model B, $\zeta_f = 1/\varepsilon$ and $\zeta_s = 0$, where $\varepsilon = \varepsilon_f$.

Standard correlations are used to evaluate the fluid-particle friction (drag). However, the drag coefficients β_M (M = A or B) depend on the model selected. According to Lyczkowski and Bouillard (1992), the relation between β_A and β_B is

$$\beta_B = \beta_A/\varepsilon \tag{5}$$

β_A is obtained from the Ergun equation (Ergun, 1952) for $\varepsilon \le 0.8$ and from Wen and Yu's (1966) correlation for $\varepsilon > 0.8$. These expressions may be summarized as follows:

For $\varepsilon \le 0.8$,

$$\beta_A = 150\frac{\varepsilon_s^2\mu_f}{\varepsilon(d_p\phi_s)^2} + 1.75\frac{\rho_g\varepsilon_s|v_f - v_s|}{d_p\phi_s} \tag{6}$$

For $\varepsilon > 0.8$,

$$\beta_A = \frac{3}{4}C_d\frac{\varepsilon\varepsilon_s\rho_f|v_f - v_s|}{d_p\phi_s}\varepsilon^{-2.7} \tag{7}$$

where,

$$C_d = \frac{24}{Re_p}\left[1 + 0.15Re_p^{0.687}\right], \text{ for } Re_p \le 1000 \tag{8}$$

$$C_d = 0.44, \text{ for } Re_p > 1000, \tag{9}$$

$$Re_p = \frac{\varepsilon\rho_g|v_f - v_s|d_p\phi_s}{\mu_f} \tag{10}$$

The particle sphericity (also called shape factor), ϕ_s, is defined as the ratio of the actual surface area of the particle to the surface area of a spherical particle of diameter d_p.

The solids elastic modules, G_s, is used to calculate the normal component of the solids stress through the relation $G_s\nabla\varepsilon$. The primary computational function of the solids stress term is to keep the bed from compacting below the defluidized of packed bed state. Any solids stress model that accomplishes this is adequate. Here we use

$$G_s = G_0\exp\left[-c(\varepsilon - \varepsilon^*)\right] \tag{11}$$

as discussed by Lyczkowski and Bouillard (1992). In this paper we use c = 600, $\varepsilon^* = 0.376$ used by Lyczkowski and Bouillard (1992). c = 500, $\varepsilon^* = 0.422$ were used by Gidaspow and Syamlal (1985). G_0 has been taken as 1.0 Pa.

The three resistance coefficients, R_i, i = x,y,z, are input to the models and can be replaced with correlations.

The gas density is determined by the ideal gas law,

$$\rho_g = \frac{\bar{M}p}{\bar{R}T} \tag{12}$$

where $\bar{M}$ is the average molecular weight, T is the absolute temperature, and $\bar{R}$ is the universal gas constant. For the fluid phase, the solids elastic modulus, G_f, is set to zero.

To solve the three-dimensional equations of fluid-solids flow given above, we need appropriate initial conditions and boundary conditions for the two phase velocities, the fluid phase pressure, and the porosity. The initial conditions depend upon the problem investigated. The inlet conditions are usually given. For example, the porosity is set to 1 where particle-free fluid enters the system. The boundary conditions at planes of symmetry demand zero normal gradient of all variables.

At an impenetrable solid wall, the fluid phase velocities in the three normal and tangential directions are set to zero. The no-slip condition cannot always be applied to the solids phase. Since the particle diameter is usually larger than the length scale of surface roughness of the rigid wall, the

particles may partially slip at the wall. This mean slip velocity is given by

$$v_s|_w = -L\frac{\partial v_s}{\partial \xi}\Big|_w \qquad (13)$$

where the ξ direction is normal to the wall, The slip parameter, L, is taken to be the mean distance between particles. In FORCE2 and FLUFIX/MOD2, the mean free path is determined by

$$L = d_p\phi_s/(6\sqrt{2}\varepsilon_s) \qquad (14)$$

Also the mean free path can be derived directly from kinetic theory of granular flow (Ding and Lyczkowski, 1992).

3. FORCE2 CODE SUMMARY

The partial differential equations with appropriate initial and boundary conditions described in the preceding section are solved by FORCE2 using the finite-difference method. The finite-difference equations are derived by dividing the flow domain into a collection of control volumes and then integrating the governing momentum and continuity equations over these volumes. This results in a set of coupled, non-linear equations describing the velocities, void fractions, and pressures within the volumes.

The flow (or computational) domain is divided into a collection of cells or control volumes in a Cartesian coordinate system. Scalar quantities such as pressure and void fraction are calculated at the centers of these volumes denoted Main Control Volumes. Fluid and solids velocities are calculated on the Main Volume faces utilizing a second set of control volumes that are "staggered" with respect to the Main Volumes. This second set of volumes connect the centers of the Main Volumes and are called Momentum Control Volumes. The collection of Main and Momentum Volumes is the conventional "staggered" mesh used in most finite-difference formulations (Patankar, 1980). A general finite-difference transport equation (representing conservation of mass or momentum) may then be derived using the general control volume arrangement as

$$a_p\phi_P = \sum a_q\phi_Q + b_p\psi_P + S_c \qquad (15)$$

where ϕ_P and ψ_P are dependent solution variables, a_q is the transport coefficients on face q of control volume P, $\sum a_q\phi_Q = a_e\phi_E + a_w\phi_W + a_n\phi_N + a_s\phi_S + a_f\phi_F + a_b\phi_B$, $a_p = \sum a_q + b_p + Sp$, S_c is a source of ϕ_P, S_P is a positive coefficient for a source of ϕ_P, and b_p is a positive coefficient linking the two dependent variables ϕ_P and ψ_P. Details about this equation can be found in Patankar's book (1980) or the FORCE2 documentation (Burge, 1991).

For transient simulations, the implicit multifield (IMF) technique (Harlow and Amsden, 1975) is used in FORCE2 and is based primarily on the IMF scheme as implemented in FLUFIX/MOD2. The solution procedure is based on adjusting the node pressure until fluid phase mass is conserved. Some key features of the method include: (1) cell-by-cell solution, (2) simultaneous solution for velocities on the cell faces, (3) explicit formulation for convection and diffusion, and (4) implicit formulation for solids stresses.

For steady-state simulations, because the finite-difference form of the momentum and continuity equations are very nonlinear, an iterative solution procedure is required. The approach is to construct sets of linear equations by evaluating the velocity, void fraction, etc., coefficients based on assumed or trial operating conditions. The resulting linear equations are solved using matrix methods and their solutions used to estimate new operating conditions. This sequence is continued until the equation residuals are small indicating that an acceptable solution has been achieved. The nonlinear nature of the governing equations also requires that the solution be advanced slowly. A key element of the solution scheme is the adjustment of the flow field pressure to conserve mass in each computational cell. The iterative procedure is based on conserving mass once a solution is achieved. The solution procedure is a modified version of SIMPLER (Patankar, 1980) developed by Schnipke (1986).

4. VALIDATION OF FORCE2

Validation of FORCE2 was identified as a key step in making the computer program a useful tool for industry and was, therefore, initiated as part the in-kind work for the Cooperative R&D Venture described in the Acknowledgments Section. Although FORCE2 is fundamentally based and, therefore, could be applied to both atmospheric and pressurized bubbling and circulating fluidized beds and liquid-solids fluidized beds and slurries, the current effort focused on validation for atmospheric bubbling gas-solids fluidized beds.

Three sources of data were selected to validate FORCE2. In the following simulations, the solids viscosity is assumed to be 0.1 Pa·s (1.0 poise) except when it is zero (inviscid solution).

4.1. FLUFIX and the FLUFIX Standard Problem

A standard problem has been formulated by ANL (Lyczkowski and Bouillard, 1992) from tests conducted at IIT (Bouillard et al., 1989) on a thin "two-dimensional" fluidized bed with an immersed obstacle located above an inlet air jet. This fluidized bed was 40 × 3.81 cm in cross-section with a central jet velocity of 5.78 m/s. The jet inlet width was 1.27 cm. A rectangular obstacle (9.74 × 2.54 cm) was placed approximately 9.74 cm above the jet. The bed material was glass beads having a particle diameter of 500 μm and a density of 2.5×10^3 kg/m^3. The initial bed height was 29.9 cm. Time-averaged porosities were obtained using a Cs-137 gamma-ray source and detected with an ionization gauge.

The FORCE2 and FLUFIX/MOD2 grid structure were developed by assuming a symmetry plane through the central jet. As a result, only half of the bed is modeled. The FORCE2 nodal structure, which was identical to that used in FLUFIX/MOD2, is depicted in Fig. 1. The predicted gas void fractions from FLUFIX/MOD2 and FORCE2 and the measured time-averaged void fractions at 10 cm and 17 cm from the center of the jet are respectively shown in Figs. 2 and 3. Instantaneous gas void fractions predicted by FLUFIX/MOD2

and FORCE in the node above the inlet jet are shown in Fig. 4. The predicted results of FORCE2 reasonably agree with the measured data and agree well with the predicted results of FLUFIX/MOD2. The agreement with the experimental data is promising and indicates that this fundamentally-based model does simulate the major hydrodynamic features of the bed.

4.2. CAPTF Three-Dimensional Fluidized Bed

A 30.5 x 30.5-cm square fluidized bed with two rows of tubes was tested in the Computer-Aided- Particle Tracking Facility (CAPTF) at the University of Illinois at Urbana-Champaign (UIUC) (Podolski et al., 1991). The bed material was glass beads with a mean particle diameter of 513 μm and a density of 2.5×10^3 kg/m^3. The initial bed height was 40.6 cm. Immersed tubes having an outer diameter of 5.08 cm were used. The bed was fluidized with a superficial air velocity of 52 cm/s. In FORCE2 model, the circular tubes were replaced by rectangular-shaped tubes, as depicted in Fig. 5.

The FORCE2 nodal structure used to simulate the bed is shown in Fig. 5. The bed is modeled in three dimensions with a total of approximately 1134 control volumes. The approximate locations of the pressure measurements (numbers 1-10 for the elevations and planes A, B, C) are also shown in Fig. 5. Figures 6 and 7 show the comparisons between measured and FORCE2 predicted power spectral densities of the pressure fluctuations located at A-10 and B-6, respectively. The frequencies of the maximum predicted power spectra at these locations approximately agree with the measured data. Neither the data nor FORCE2 indicate pronounced three-dimensional effects. The measured and predicted power spectrum at various elevations did not vary significantly from plane to plane (Burge, 1991). Based on these predictions, FORCE2 provided a reasonable simulation of the 3-D CAPTF tube bundle.

4.3. Foster Wheeler Half-Depth Tube Bundle

A series of pressure fluctuation and erosion tests were conducted by the Foster Wheeler Development Corporation (FWDC) on a two-row tube bundle in a bubbling fluidized bed (Podolski et al., 1991). Pressure fluctuation data collected during testing of the 76.2 cm deep (called the half-depth bundle) bed were used for the validation study here. The mean particle diameter was 1500 μm. The particle density was 1.28×10^3 kg/m^3. The initial bed height was 40.64 cm. The inlet air fluidizing velocity was 121.9 cm/s.

In the FORCE2 model, quarter-symmetry is assumed at the mid-width and mid-depth of the bed. The nodal structure is shown in Fig. 8. The computed pressure time series of 1100 points were used to determine the power spectral densities. Computed and measured power spectral of pressure fluctuations at locations A-2 and B-2 are shown in Figure 9 and 10, respectively.

The predicted and the measured major frequencies compare favorably. Predicted and measured maximum powers occur in different planes, as shown in Fig. 11. This indicates the three-dimensional effects in the bed.

5. CONCLUSIONS

The three-dimensional hydrodynamic computer code FORCE2 for fluid-solids flow has been developed at B & W in close collaboration with ANL. Applications of FORCE2 in atmospheric gas-solids fluidized beds have been successfully carried out as demonstrated in this paper. Favorable comparisons with data have been shown and indicate that the models and modeling approach are sound. Many features, such as three dimensions, variable control volume size, flow resistance coefficients, and volume porosities and surface permeabilities, needed to model industrial-scale fluidized beds, have been included into FORCE2. With our three-dimensional hydrodynamic computer code FORCE2, it is now possible to better model complex large-scale fluid-solids systems including atmospheric and pressurized bubbling and circulating fluidized bed combustors gasifiers and incinerators and slurries for many industrial applications.

ACKNOWLEDGMENTS

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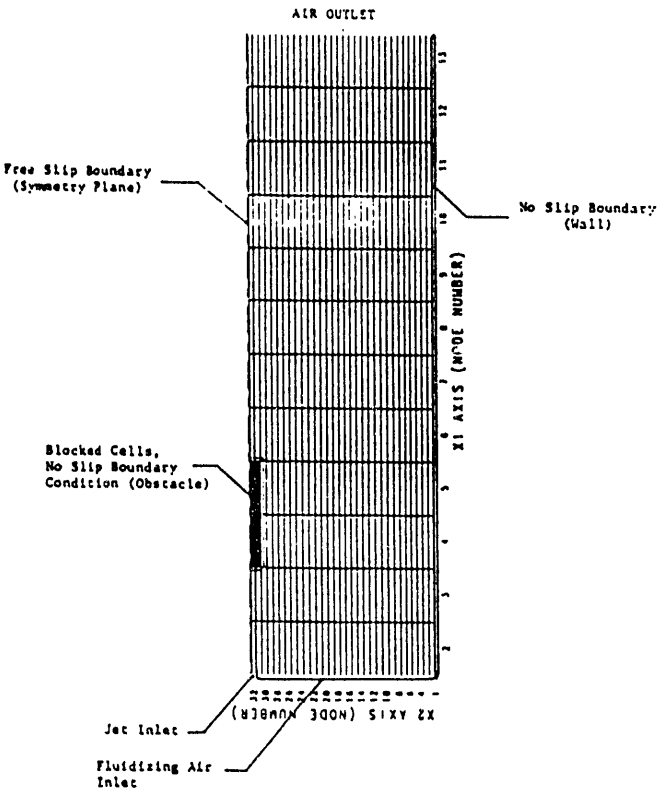


FIGURE 1. FORCE2 NODAL STRUCTURE USED FOR THE SOLUTION OF THE STANDARD PROBLEM

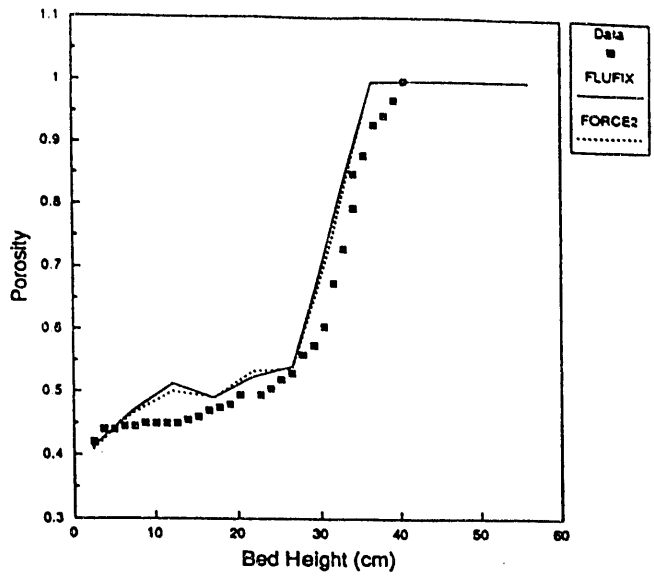


FIGURE 2. PREDICTED AND MEASURED TIME-AVERAGED BED POROSITIES 10 cm FROM THE CENTER OF THE JET, INVISCID SOLUTION ($\mu_S = 0$)

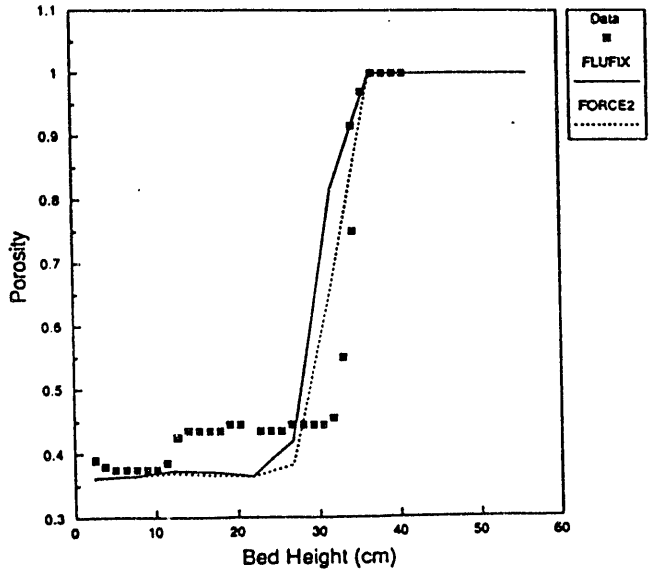


FIGURE 3. PREDICTED AND MEASURED TIME-AVERAGED BED POROSITIES 17 cm FROM THE CENTER OF THE JET, INVISCID SOLUTION ($\mu_S = 0$)

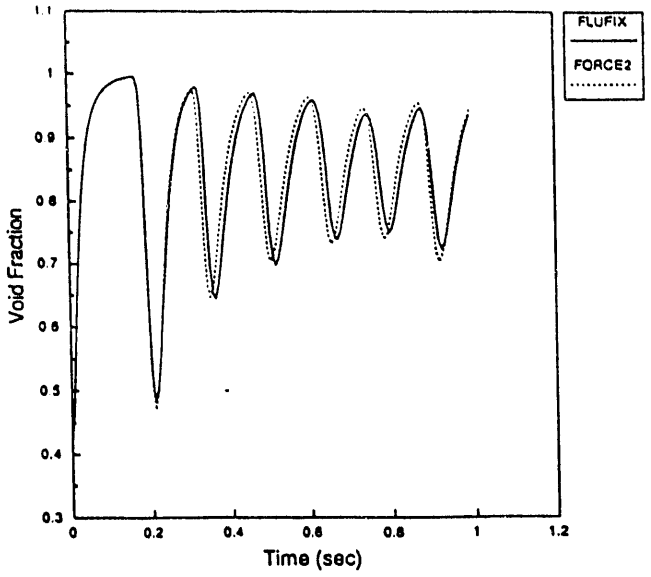


FIGURE 4. INSTANTANEOUS GAS VOID FRACTION PREDICTED BY FLUFIX AND FORCE2 IN THE NODE ABOVE THE JET, VISCOUS SOLUTION (μ_S = 0.1 Pa·s)

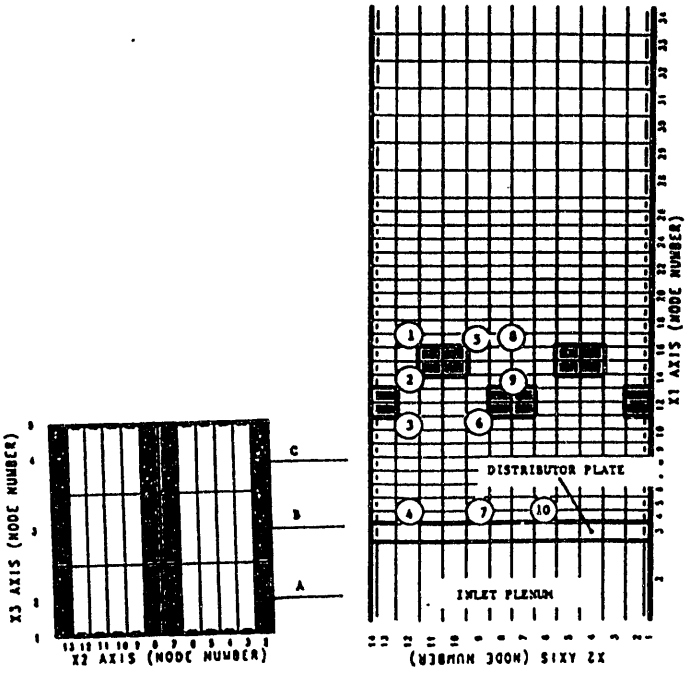
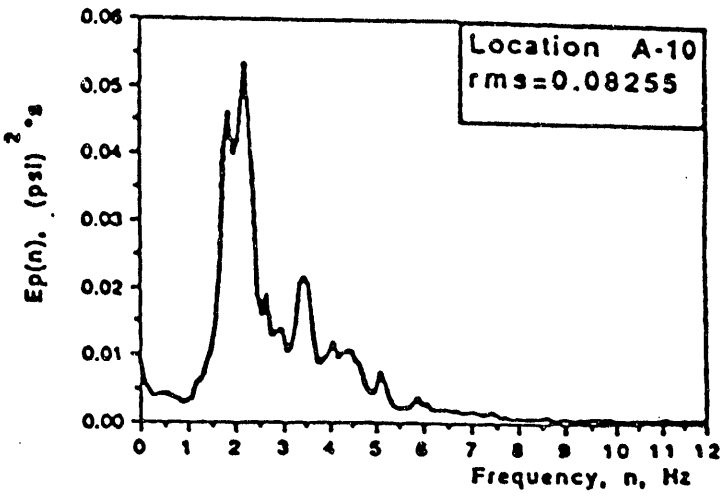


FIGURE 5. FORCE2 NODAL STRUCTURE USED TO MODEL THE 30.5 x 30.5-cm SQUARE FLUIDIZED-BED TUBE BUNDLE TESTED IN THE CAPTF



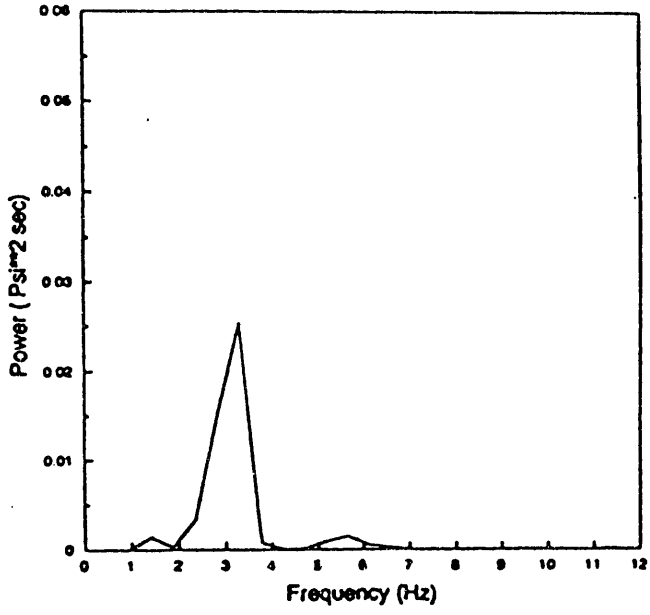
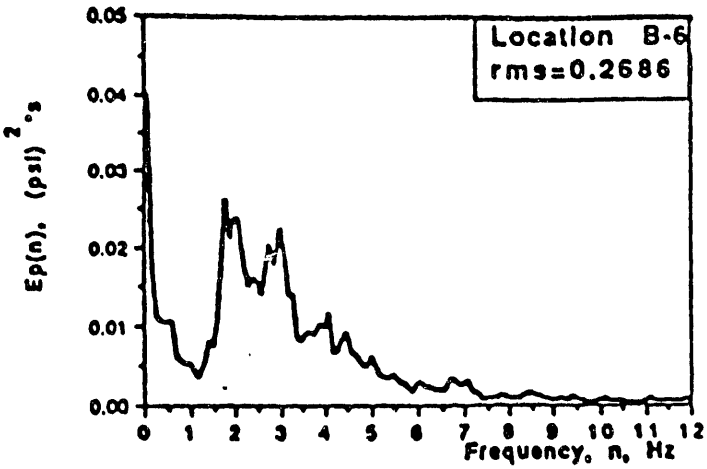


FIGURE 6. PREDICTED (LOWER) AND MEASURED (UPPER) POWER SPECTRAL DENSITIES OF THE PRESSURE FLUCTUATIONS IN THE 30.5 x 30.5-cm SQUARE CAPTF TUBE BUNDLE, LOCATION A-10



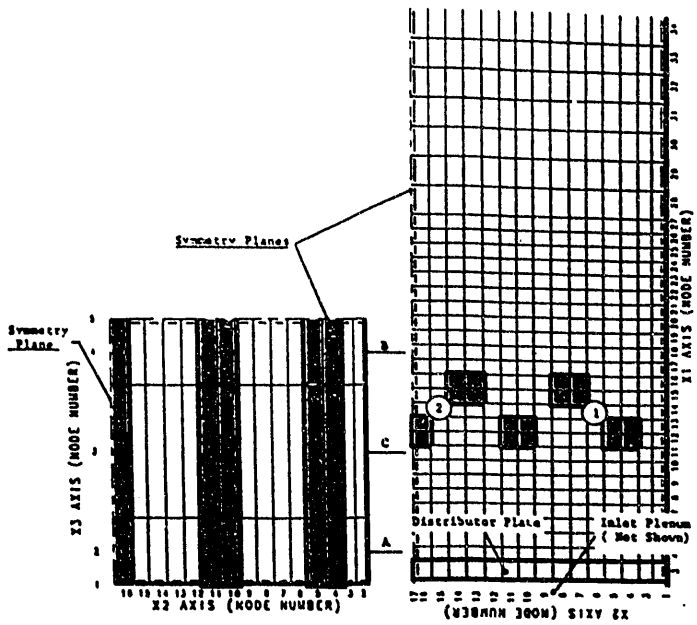


FIGURE 8. FORCE2 NODAL STRUCTURE USED TO MODEL THE FWDC HALF-DEPTH TUBE BUNDLE

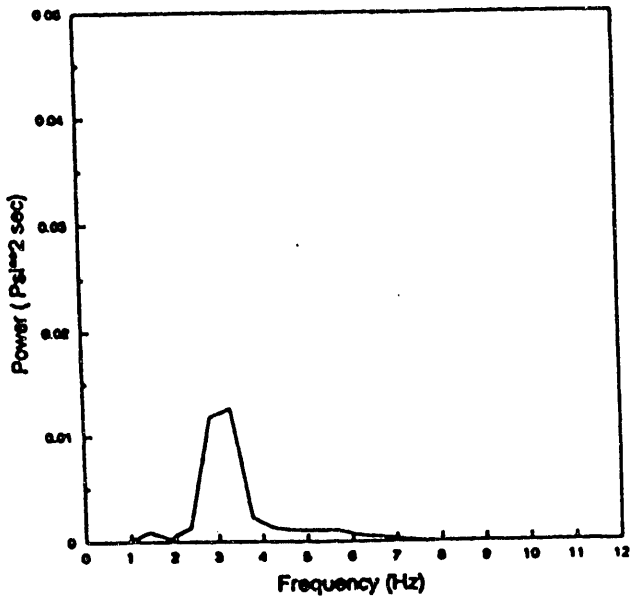


FIGURE 7. PREDICTED (LOWER) AND MEASURED (UPPER) POWER SPECTRAL DENSITIES OF THE PRESSURE FLUCTUATIONS IN THE 30.5 x 30.5-cm SQUARE CAPTF TUBE BUNDLE, LOCATION B-6

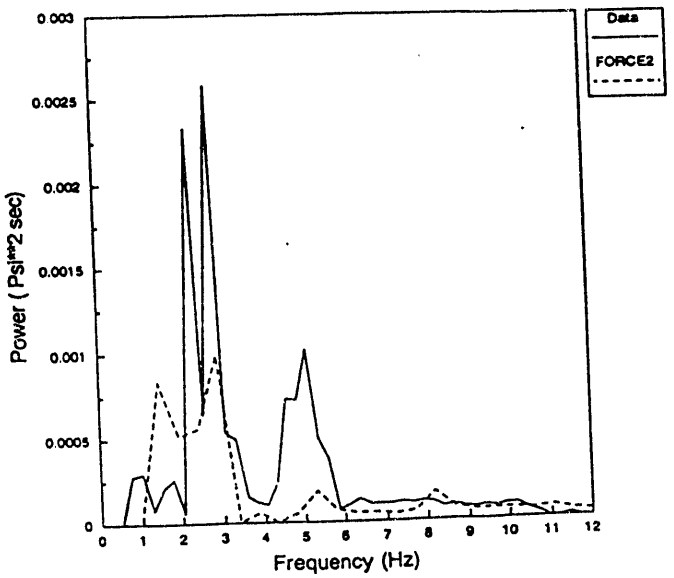


FIGURE 9. PREDICTED AND MEASURED POWER SPECTRAL DENSITIES OF THE PRESSURE FLUCTUATIONS IN THE FWDC HALF-DEPTH TUBE BUNDLE, LOCATION A-2

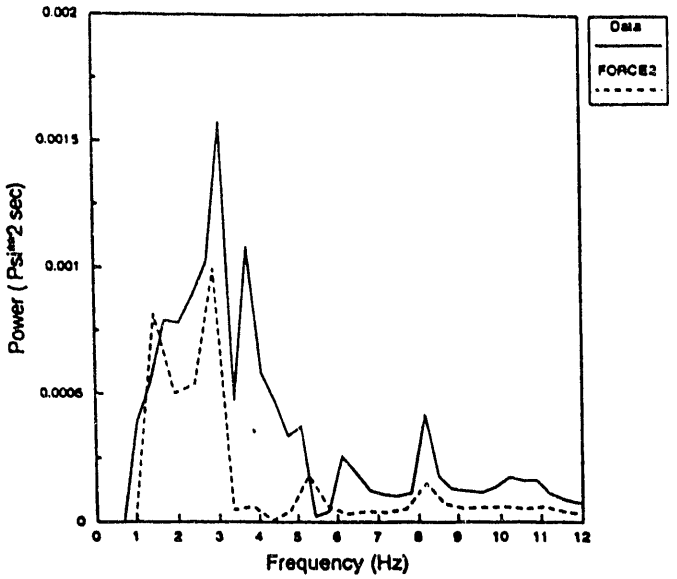


FIGURE 10. PREDICTED AND MEASURED POWER SPECTRAL DENSITIES OF THE PRESSURE FLUCTUATIONS IN THE FWDC HALF-DEPTH TUBE BUNDLE, LOCATION B-2

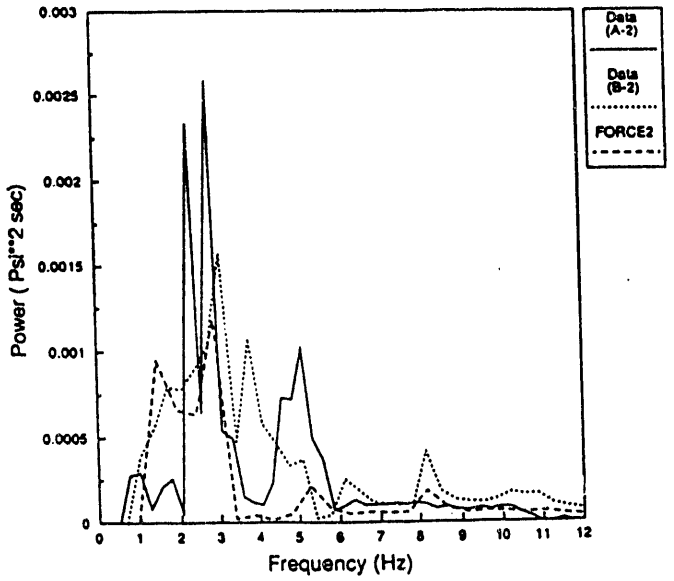


FIGURE 11. PREDICTED AND MEASURED POWER SPECTRAL DENSITIES OF THE PRESSURE FLUCTUATIONS IN THE FWDC HALF-DEPTH TUBE BUNDLE, LOCATIONS C-2 (PREDICTED) AND LOCATIONS A-2 AND B-2 (MEASURED)

END

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