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ATOMIC ENERGY OF CANADA LIMITED

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INTEGRATED AEROSOL AND THERMALHYDRAULICS MODELLING FOR CANDU® SAFETY ANALYSIS

MODÉLISATION INTÉGRÉE DE PHÉNOMÈNES RÉGISSANT LES AÉROSOLS ET LA THERMOHYDRAULIQUE POUR L'ANALYSE DE SÛRETÉ DES RÉACTEURS CANDU®

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RÉSUMÉ

L'analyse d'accidents hypothétiques dans les réacteurs CANDU, lesquels pourraient entraîner de graves dégâts de combustible, demande qu'on puisse modéliser la formation d'aérosols contenant des produits de fission ainsi que la migration de ces aérosols du combustible à une fuite quelconque dans l'atmosphère en passant par l'enceinte de confinement. Les calculs de la valeur optimale demandent le couplage étroit et la résolution simultanée de toutes les équations décrivant toute la gamme de phénomènes physiques et chimiques en jeu. On a réalisé le prototype CATHENA/PACE-3D pour le calcul intégré de phénomènes régissant les aérosols et la thermohydraulique d'un réacteur CANDU au cours d'accidents hypothétiques. Des exemples démontrent la capacité de CATHENA/PACE-3D de donner des régimes réalistes d'écoulement et de circulation et une exactitude convenable de résolution de deux cas simples d'essai d'écoulement de fluide pour lesquels il existe des solutions analytiques.

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ABSTRACT

Analysis of postulated accidents in CANDU reactors that could result in severe fuel damage requires the ability to model the formation of aerosols containing fission product materials and the transport of these aerosols from the fuel, through containment, to any leak to the atmosphere. Best-estimate calculations require intimate coupling and simultaneous solution of all the equations describing the entire range of physical and chemical phenomena involved. The prototype CATHENA/PACE-3D has been developed for integrated calculation of thermalhydraulic and aerosol events in a CANDU reactor during postulated accidents. Examples demonstrate the ability of CATHENA/PACE-3D to produce realistic flow and circulation patterns and reasonable accuracy in solution of two simple fluid-flow test cases for which analytical solutions exist.

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1. INTRODUCTION

For proper analysis of postulated accidents in CANDU®* reactors that could result in severe fuel damage, it is essential to be able to model the formation of aerosols containing fission product materials and the transport of these aerosols from the fuel channels, through the reactor cooling system, to any breach into containment and then to any potential leak to the outside atmosphere. This radioactive "source term" to the public is perhaps the major consequence of any reactor accident.

In recent years, it has become increasingly clear that the analysis of nuclear aerosol behaviour cannot be decoupled from analysis of the local thermalhydraulics either in the cooling system or in containment [1,2]. Major phenomena that must be considered during analysis of severe-fuel-damage accidents are depicted in Figure 1. Analysis of the sequence of events following a postulated accident, in which reactor fuel elements are damaged and fission product materials are released, can be subdivided into two: analysis of phenomena in the primary circuit, and the containment building.

In the primary circuit, one-dimensional analysis is believed to be adequate because CANDU reactors use a pressure tube design. Steam pressures, temperatures and flows will influence the condensation of vapours released from the fuel assemblies at high temperatures to form aerosols of structural materials, uranium oxide and fission products. The transport and deposition of the aerosol materials throughout the pipework of the primary circuit will also depend on steam flow, pressure and temperature. In turn, the quantity of deposited materials will affect flow paths, and decay heat generated by the deposits could result in elevated metalwork and carrier gas temperatures. Thermalhydraulics and aerosol behaviour are thus intimately related and cannot realistically be separated if code results are to be credible.

In containment, a three-dimensional analysis is required because hydrogen, steam and aerosol distributions will be determined by flow circulation and gas and particulate mixing. Steam condensation on wet aerosol materials, and evaporation of water from such aerosols, will be determined by local carrier gas pressures and temperatures, as well as by local aerosol chemical and decay heat releases. Combustion events will affect aerosol behaviour by means of the thermalhydraulic responses to such events. Thus, best-estimate calculations of fission product transport require intimate coupling, and simultaneous solution, of all the equations describing the entire range of physical and chemical phenomena involved.

We have begun to assemble computer codes that we will eventually use in a fully coupled fashion to address all aspects of fission product transport in CANDU reactors. Initially, we have chosen to focus on the coupling of thermalhydraulics and aerosol physics, and, to this end, we have begun to use the CATHENA [3] and PACE [2] codes in a fully integrated

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* CANada Deuterium Uranium. Registered in the U.S. Patent and Trademark Office.

fashion (see Figure 2). To provide the means of calculating containment behaviour, we have extended the capability of this code package to perform calculations in three dimensions. (CATHENA, the Canadian Algorithm for THErmalhydraulic Network Analysis, is a two-fluid thermalhydraulics code designed specifically to calculate heat and fluid flow for CANDU cooling systems, and PACE, a Program for Aerosol Code Evaluation, has been developed based on existing aerosol physics codes to provide a tool for analysis of fission product aerosol behaviour.)

The CATHENA/PACE code, in prototype form, has been used successfully for simulating high-temperature experiments designed to establish the rates of aerosol material production from unirradiated CANDU fuel samples. During these experiments, the samples are held at about 2000°C for about 10 min in a flowing steam atmosphere. The exothermic metal-water reaction must be simulated properly to get the correct sample heat-up rates and, consequently, the correct aerosol release. Calculated aerosol transport results using the coupled CATHENA/PACE code are consistently within about 10% of the experimental measurements over a variety of test conditions. Results of these exercises will be made available in forthcoming publications.

This report begins with a brief review of the one-dimensional CATHENA/PACE code for best-estimate calculation of aerosol events in the primary circuit of a CANDU reactor during postulated severe-fuel-damage accidents. The focus then shifts to the three-dimensional model that has recently been incorporated to extend our computational capability to aerosol events in containment as well. An example is given to demonstrate that the three-dimensional prototype code (CATHENA/PACE-3D) is able to produce realistic flow and circulation patterns at typical containment pressure and temperature accident conditions. Reasonable accuracy of the prototype CATHENA/PACE-3D is demonstrated in two simple test cases for which analytical solutions exist.

2. GOVERNING AEROSOL EQUATIONS

We begin the review of the aerosol model incorporated in CATHENA/PACE by examining the basic equation that must be solved in obtaining a solution to primary circuit aerosol transport and deposition processes. In general, one divides the core and the primary circuit into connected control volumes within which the aerosol and carrier gas atmosphere are assumed to be well mixed. This means that there are no differences from point-to-point within the control volume in carrier gas properties or aerosol particle sizes or concentrations. All gradient information is lost. (Some of it must be empirically reconstructed to prescribe particle removal rates.) All new aerosol particles introduced into the control volume are assumed to be instantly and uniformly distributed throughout. In some cases, in particular with large control volumes, the assumption of homogeneous mixing could be considered an oversimplification of the real problem. The major advantage of the well-mixed aerosol assumption is that it reduces an extremely complex physical problem to a fairly simple one.

One may consider these connected control volumes to represent actual primary circuit components and use gas flow velocity data to transport aerosols from one volume to the next (the Eulerian approach), or one may consider that these volumes are packets of gas and particles that "go with the flow" (the Lagrangian approach). The Eulerian approach is generally simpler and faster but less accurate than the Lagrangian.

For a single aerosol species, a single conservation equation, of integro-differential form, is used for problem description [4]:

$$\frac{\partial}{\partial t} C(m,x,t) + \frac{\partial}{\partial x} [v(m,x,t)\, C(m,x,t)] =$$
$$\frac{1}{2} \int_0^m d\mu\ \phi(\mu, m-\mu)\, C(\mu,x,t)\, C(m-\mu,x,t) - C(m,x,t) \int_0^\infty d\mu\ \phi(\mu,m)\, C(\mu,x,t)$$
$$- \frac{\partial}{\partial m} [\xi(m,x,t)\, C(m,x,t)] - R(m,x,t)\, C(m,x,t) + S(m,x,t) \qquad (1)$$

where $C(m,x,t)$ is the number of particles of mass m at distance x in the primary circuit at time t. The first term on the left of this equation prescribes the time rate of change of $C(m,x,t)$ and the second term on the left prescribes the gradient of the flux of $C(m,x,t)$ along the primary circuit in the x direction, where $v(m,x,t)$ is aerosol particle velocity.

The first two terms on the right, the integrals, describe the process whereby small particles agglomerate to form larger ones. In the first term, all particles that combine to form new particles of mass m are added. The agglomeration kernel, $\phi(\mu, m-\mu)$, prescribes the rate at which particles of masses μ and $m - \mu$ combine to produce particles of mass m. The coefficient 1/2 is needed because the integral counts each agglomeration twice. In the second term, all particles of mass m that combine with all other particles through agglomeration are subtracted. In the third term, the growth of particles due to condensation of steam is prescribed. The condensation rate is $\xi(m,x,t)$. In the fourth term, the removal rate $R(m,x,t)$ describes the rate at which particles of mass m are removed from the atmosphere by deposition on structural surfaces or by leakage to the environment. The last term represents new particles of mass m injected into the atmosphere at the rate $S(m,x,t)$.

To emulate those aerosol codes that have true multicomponent capability, it is necessary to specify an equation like Equation (1) for each component. If $q_k(m,x,t)$ is the mass of component k in particles of mass m at distance x along the primary circuit at time t, the multicomponent aerosol population balance equation, analogous to Equation (1), is

$$\frac{\partial}{\partial t} q_k(m,x,t) + \frac{\partial}{\partial x} [v(m,x,t)\, q_k(m,x,t)] =$$
$$\int_0^m d\mu\ \phi(\mu, m-\mu)\, q_k(\mu,x,t)\, C(m-\mu,x,t) - q_k(m,x,t) \int_0^\infty d\mu\ \phi(\mu,m)\, C(\mu,x,t)$$
$$+ \delta_{ik} \xi_k(m,x,t)\, C(m,x,t) - \frac{\partial}{\partial m} [\xi_k(m,x,t)\, q_k(m,x,t)]$$
$$- R(m,x,t)\, q_k(m,x,t) + S_k(m,x,t) \quad . \qquad (2)$$

Here C(m,x,t) remains the total number of aerosol particles of mass m. If there are L species,

$$\sum_{k=1}^{L} q_k(m,x,t) = m\, C(m,x,t) \quad . \tag{3}$$

All terms are equivalent to those preceding, except for the term $\delta_{ik}\xi_k(m,x,t)\, C(m,x,t)$. The Kronecker delta function δ_{ik} is unity when k = i, defined as the condensing (or evaporating) component, and is zero for other components. This term corresponds to the change in the airborne mass of this component. In other words, it defines the condensation of vapour of component k on aerosol particles of mass m and is separate from the familiar differential term that corresponds to the shifting of mass up (or down) the mass range due to condensation (or evaporation) [4]. (The reader may have noticed the similarity in form between the $\partial/\partial m$ and the $\partial/\partial x$ terms in these equations and wondered if the Eulerian/Lagrangian approach considerations might apply to condensation modelling as they do to physical aerosol transport. They do.) PACE incorporates the multi-component Equation (2).

3. THE CATHENA/PACE PROTOTYPE CODE

To facilitate the comparison of the effects of the various aerosol model assumptions, a simple finite-difference code has been built that permits, by switch selection, emulation of aerosol physics models from other state-of-the-art aerosol codes (e.g., HAA4, REMOVAL, NAUA, AEROSIM, CONTAIN/MAEROS, AEROSOLS/B1, RAFT, VICTORIA, TRAP-MELT). This code is called PACE [4,5], and, in its basic form, requires thermalhydraulic conditions to be provided as input data. While all integrations are done numerically, an equivalent lognormal distribution at each time step is selectable. Thus, virtually all the major possibilities are available. The numerical method chosen was the Method of Weighted Residuals [6], in a finite difference formulation with parameters chosen to match AEROSIM [5]. Semi-implicit backward Euler integration was used to advance the solution in time, with automatic time-step control as used in the thermalhydraulics code CATHENA [3]. Following the documentation available for the particular codes emulated in PACE, all variations for agglomeration, removal and condensation were modelled. Thus, by specifying the code-to-be-emulated as input data, the appropriate models are automatically selected. Override selection of parameters such as those in the collision efficiency model, wet or dry aerosols, or Stephan flow model, permits emulation of many variations. In cases where the available documentation is unclear about model selection, CONTAIN/MAEROS models were used [7].

The PACE code itself is strictly an aerosol behaviour model and does not incorporate any aerosol-thermalhydraulics interaction. Thus it cannot really emulate the performance of CONTAIN (for example), which does include a full containment thermalhydraulics package. PACE simply distributes condensing vapour over the aerosol particles, and the method used is that reported for AEROSIM [4].

CATHENA [3] was developed for specific calculation of CANDU primary circuit thermalhydraulic response during accident conditions. It uses a node-link representation for the primary circuit and has two-fluid capability as well as a sophisticated heat transfer package for calculation of temperature transients in CANDU fuel channels during accident conditions.

PACE has been coupled to CATHENA to provide integrated analysis. At each time step (controlled by CATHENA), thermalhydraulic data are passed to PACE subroutines, which calculate the local aerosol physics response, and PACE returns to CATHENA any specific results that will have impact on the thermalhydraulic calculations for the next time step. The CATHENA/PACE code strategy is shown in Figure 2.

4. THE CATHENA/PACE-3D PROTOTYPE CODE

The main reason for producing a three-dimensional code is the need to model gas and aerosol mixing in containment, where the assumptions of either large well-mixed volumes or one-dimensional flow are inadequate. A similar need exists for modelling fission-product aerosol transport through CANDU headers. Since aerosol transport has already been integrated with CATHENA (through the PACE code), it makes sense to produce a three-dimensional capability for CATHENA.

CATHENA is a node-link code based on the concept of branches. A branch is usually viewed as being a pipe (i.e., a one-dimensional element) consisting of several nodes connected together in series, with the right end of the first node connected to the left end of the second node by a link, and so on. Ends of branches may be connected together to form networks. Such interbranch connections are also called links. Mass (continuity) and energy conservation equations are written for each node, and equations of motion (or momentum) are written for each link in a CATHENA network.

As a first step to multidimensionality, consider dividing a branch into several parallel sub-branches with parallel flows. To assist in this exercise, first consider the parallel branches to be concentric cylinders in a pipe of circular cross section. The innermost cylindrical flow will experience drag due to the flow in the adjacent (outer) cylinder. The outermost cylindrical flow will experience drag due to the flow in the adjacent (inner) cylinder and due to the pipe wall (zero flow). Now, consider modelling the drag forces for adjacent cylindrical flows as being identical to those that would arise from moving pipe walls. All that becomes required is to keep track of which flows are adjacent to each other and to adjust the equivalent hydraulic diameters to reflect correctly the flow geometries. The same principle may be applied to non-concentric flows. Viscous drag effects will be automatically accounted for in the same way, and to the same level of accuracy, as they are currently handled in the single "flow in a pipe" case. This relatively simple approach has been used for CATHENA/PACE-3D and represents an approximation for solution

of the Navier-Stokes equations of motion. The efficacy of this simplification will be examined subsequently.

Conceptually then, for CATHENA/PACE-3D, we are considering a set of parallel branches with parallel flows to represent axial flow through some physical component (for example, through a "thick" pipe). We let these flows interact in that we let them drag each other. To complete the multidimensional flow picture, we have to introduce cross-flow.

We define axial flow as being in the z direction. Subroutines in CATHENA will have already written all the axial momentum equations, as they have come directly from the several "z-branch" links. This statement is the key to the three-dimensional algorithm: because specifying the several parallel branches in the z-direction leads directly within CATHENA to the z-direction momentum equations, we can get CATHENA to generate automatically all the x- and y-direction momentum equations for cross-flows simply by specifying x- and y-direction branches that connect the CATHENA nodes in the cross-flow directions.

5. MATHEMATICAL REPRESENTATIONS FOR CATHENA/PACE-3D

CATHENA/PACE-3D numerical models for the conservation laws in three dimensions are based on straightforward extensions of the mass and energy conservation laws currently handled within the CATHENA [8] one-dimensional framework, and in the writing of the additional transverse-flow momentum (or Navier-Stokes) equations.

To begin with, in three dimensions, the continuity equation for single-phase flow is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \, \underline{v}) = 0 \qquad (4)$$

where ρ is the fluid density and $\underline{v}$ is the fluid velocity vector. (The fluid could be either liquid or vapour or a homogeneous two-phase mixture. For extension to two-fluid representation, see Reference 3). Expanding the velocity vector in Cartesian coordinates we obtain

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho \, v_x) + \frac{\partial}{\partial y} (\rho \, v_y) + \frac{\partial}{\partial z} (\rho \, v_z) = 0 \quad . \qquad (5)$$

When there is only z-directional flow, we get the familiar one-dimensional equation that is differenced in CATHENA [8]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z} (\rho \, v_z) = 0 \quad . \qquad (6)$$

Treatment of the mass (and, similarly, the energy) conservation equation in the extension of CATHENA/PACE to CATHENA/PACE-3D simply

involves adding the mechanisms for accumulating the contributions at each control volume for the transverse flows, which are the additional terms:

$$\frac{\partial}{\partial x}(\rho\, v_x) \text{ and } \frac{\partial}{\partial y}(\rho\, v_y) \quad .$$

Treatment of momentum is somewhat more complex. In CATHENA/PACE, a single, one-dimensional momentum equation is written, whereas in CATHENA/PACE-3D, three momentum conservation equations are written, one for each coordinate direction. The component of momentum in the n direction (with $\underline{n}$ being the unit vector in the n direction) is

$$\frac{\partial}{\partial t}(\rho\, v_n) + \nabla\cdot(\rho\, v_n\, \underline{v}) = -\underline{n}\cdot\nabla p + \mu\, \nabla^2 v_n + F_n \qquad (7)$$

where v_n is the velocity in the n direction, p is pressure, μ is viscosity, and F_n is the body force in the n direction.

Expanding the n-direction momentum equation and making use of the continuity equation results in the form of momentum equation differenced in CATHENA/PACE-3D:

$$\rho\left(\frac{\partial v_n}{\partial t} + \underline{v}\cdot\nabla v_n\right) = -\underline{n}\cdot\nabla p + \mu\, \nabla^2 v_n + F_n \qquad (8)$$

which may be identified as the n-direction Navier-Stokes equation. For example, if "z" is the n direction, we have the equation differenced in CATHENA/PACE-3D, using standard CATHENA methods:

$$\frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} = \frac{1}{\rho}\left(-\frac{\partial p}{\partial z} + \mu\, \nabla^2 v_z + F_z\right) \quad . \qquad (9)$$

This is the equation of motion used for <u>each</u> coordinate direction in CATHENA/PACE-3D. Note that in the case where there is <u>only</u> z-directional flow, we get the familiar one-dimensional equation differenced in CATHENA [8]:

$$\frac{\partial v_z}{\partial t} + v_z \frac{\partial v_z}{\partial z} = \frac{1}{\rho}\left(-\frac{\partial p}{\partial z} + \mu\, \nabla^2 v_z + F_z\right) \qquad (10)$$

Comparing Equations (9) and (10), we note that the transverse "acceleration" terms

$$v_x \frac{\partial v_z}{\partial x} \text{ and } v_y \frac{\partial v_z}{\partial y}$$

have been accounted for [9] in the three-dimensional formulation.

In CATHENA/PACE, the term $\mu\, \nabla^2 v_z$ is handled by specifying an equivalent friction factor for one-dimensional flow in a duct. For the

three-dimensional case, we choose to view the "duct" as having moving walls; that is, a wall segment could either be a fixed surface (as in usual one-dimensional flow) or a surface moving in the same coordinate direction at the velocity of the fluid in an adjacent control volume (for two- or three-dimensional representation). This is actually done in CATHENA/PACE-3D for <u>each</u> of the two phases defining the two-fluid model.

To be specific, in CATHENA, the wall shear force per unit flow area for the "mixed" flow regime is [3]

$$\tau_{kw} = -\zeta_k \left[\frac{\tau^* f_{kw}}{D_e} \rho_k |v_k| \frac{v_k}{2} + (k/l) \rho_m |v_m| \frac{v_m}{2} \right] \tag{11}$$

where ρ_m is the mixture density, v_m is the mixture velocity, and ζ_k, τ^*, f_{kw}, D_e, and (k/l) are the wall shear portion for phase k, the two-phase friction-factor multiplier, the phase k wall-friction factor, the conduit hydraulic diameter, and the minor loss coefficient respectively. (Note that f_{kw} may depend upon v_k.)

In CATHENA/PACE-3D, the factor τ_{kw} is written for z-directional flow and incorporated in the shear expression representing $\mu \nabla^2 v_z$ in the z-direction momentum equation, for x-directional flow and incorporated in the x-direction momentum equation, and also for y-directional flow and incorporated in the y-direction momentum equation, as follows.

Consider z-directional flow in a node (actually along links connecting nodes). The perimeter of the flow area may consist strictly of motionless hard surfaces or of adjacent nodes with their own z-direction flows, as shown in Figure 3. The hydraulic diameter for CATHENA/PACE-3D node calculations is determined as follows, with reference to Figure 3. The wetted perimeter around the surface A, S, is calculated as usual,

$$S = \sum_i S_i \tag{12}$$

and the hydraulic diameter follows,

$$D_e = \frac{4A}{S} \quad . \tag{13}$$

Note that a "parallel" connection has been imposed,

$$\frac{1}{D_e} = \frac{S}{4A} = \sum_i \frac{1}{D_{ei}} \tag{14}$$

where $De_i = 4A/S_i$.

For shear calculation purposes, the phase velocity normal to the surface A, v_k, is determined as,

$$v_k = \sum_i \frac{S_i}{S}(v_k - v_{ki}) \quad . \tag{15}$$

With these definitions, the Navier-Stokes equations for fully three-dimensional flow are calculated in CATHENA/PACE-3D, producing results that are consistent in level of detail and accuracy with the one-dimensional analysis in CATHENA. Finally, the multicomponent aerosol mass balance equation in three dimensions, written at vector location $\underline{x}$, is

$$\begin{aligned} &\frac{\partial}{\partial t} q_k(m,\underline{x},t) + \nabla\cdot[\underline{v}(m,\underline{x},t)\, q_k(m,\underline{x},t)] = \\ &\int_0^m d\mu\ \phi(\mu,m-\mu)\, q_k(\mu,\underline{x},t)\, C(m-\mu,\underline{x},t) - q_k(m,\underline{x},t) \int_0^\infty d\mu\ \phi(\mu,m)\, C(\mu,\underline{x},t) \\ &+ \delta_{ik}\xi_k(m,\underline{x},t)\, C(m,\underline{x},t) - \frac{\partial}{\partial m}[\xi_k(m,\underline{x},t)\, q_k(m,\underline{x},t)] \\ &- R(m,\underline{x},t)\, q_k(m,\underline{x},t) + S_k(m,\underline{x},t) \end{aligned} \tag{16}$$

where all terms remain as they were defined at Equation (2).

A two-dimensional version of this model has also been developed and is known as CATHENA/PACE-2D.

6. A 3 BY 3 BY 3 SAMPLE CALCULATION USING CATHENA/PACE-3D

An example is appropriate at this stage to demonstrate the potential of three-dimensional analysis for containment thermalhydraulics. Let us consider a 3-m-high tank with a rectangular section of side 1.5-m, which we represent for CATHENA/PACE-3D analysis as a 3 by 3 by 3 node system. Figure 4 shows a schematic view of the test-case geometry. Flow enters steadily at 25 g/s from a horizontal pipe near the bottom (this inflow could be considered to be a jet that impinges on the far inner surface of the tank). This demonstration case is run with steam flow only, and without any aerosols present. Flow patterns in the bottom, middle, and upper slices of the tank, at the surfaces between the nodes are shown in Figures 5, 6 and 7 respectively. The patterns demonstrate the expected symmetries and recirculations, and show that CATHENA/PACE-3D is able to present a realistic picture of flow phenomena in such geometries.

7. ANALYTICAL TEST PROBLEMS

To examine the accuracy of this three-dimensional model in more detail, we consider two fluid-flow test cases in two dimensions that have analytical solutions. The first of these relates to the contact of the jet with the wall in the previous example, and the second relates to behaviour at the jet entrance to the tank in the previous example.

It must be stated at the outset that the testing and validation of a multidimensional flow simulation code is a formidable task. The first step in the testing of the prototype CATHENA/PACE-2D code has focused on demonstrating that the numerical methods used provide a converged solution to the Navier-Stokes equations. The test problems should exercise the fundamental aspects of the code, such as flow at various angles to the computational grid system and the viscous interactions between adjacent flows or a wall. The prototype version does not include turbulence modelling, and for this reason, initial testing has focused on laminar flow for problems where analytical solutions exist to the Navier-Stokes equations.

As a first step we have examined two-dimensional laminar flows because this tests the same code structure as a three-dimensional case and allows a much broader base of "exact" analytical solutions. The two test problems chosen were 1) planar, two-dimensional flow into a stagnation point, and 2) developing flow in the inlet of a channel.

Flow into a Stagnation Point

The test problem definition is shown in Figure 8 with the coarsest CATHENA/PACE-2D simulation grid. The flow is symmetric about the stagnation line and therefore only the right-hand side of the solution domain has been simulated. The boundary conditions used in the CATHENA/PACE-2D simulations were as follows:

1) uniform flow downward at the upper boundary,

   $v = U$ along $y = 1$,

2) constant pressure at the right-hand boundary,

   $P = C$ along $x = 1$,

3) zero flow through the stagnation line,

   $u = 0$ along $x = 0$, and

4) zero flow through and along the lower boundary,

   $u = 0$ and $v = 0$ along $y = 0$.

The constant-pressure boundary condition along the $x = 1$ outlet was chosen for convenience. The dynamic pressure variation across the boundary layer, however, is small since the velocities are small.

An exact solution of the two-dimensional Navier-Stokes equations for the planar flow into a stagnation point follows from Milne-Thomson [10]. The velocity components for the flow field are given by

$$u(x,y) = u_p(x)F' \quad ; \quad v(x,y) = v_p(y) + U(\eta - F)/R^{0.5}$$

where $u_p(x) = Ux/a$ and $v_p(y) = -Uy/a$

$\eta = y\sqrt{R}$ and $R = \frac{U}{a\nu}$

U ≡ free stream velocity far from the stagnation point,

a ≡ dimension of the cavity,

$\nu = \mu/\rho$ ≡ kinematic viscosity,

and the functions F and F′ are obtained from the solution of the ordinary differential equation

$$F''' + FF'' + 1 - F'^2 = 0$$

with boundary conditions

$$F(0) = F'(0) = 0 \text{ and } F'(\infty) = 1 \quad .$$

The CATHENA/PACE-2D simulations were performed with water as the fluid at 20°C and at atmospheric pressure ($\rho \simeq 1000$ kg/m^3). To make the growth of the boundary layer from the stagnation point clearly visible, an artificially large dynamic viscosity (μ = 3 kg/m•s) was used. The flow boundary condition for the velocity was U = 1 x 10^{-2} m/s.

Three simulations were performed refining the computational grid. The coarsest grid used was a 4 by 4 grid, an intermediate 8 by 8 grid was then used and finally a 12 by 12 grid simulation was performed. The velocity field resulting from these simulations are compared with analytical solution in Figures 9 through 11. The comparison in these figures is in the form of velocity vectors drawn from the centre of each grid location for both the analytical and CATHENA/PACE-2D solution. The solid arrow head represents the analytical solution.

The comparison demonstrates that the CATHENA/PACE-2D flow field is converging towards the analytical flow field as the grid is refined. It is also encouraging to note that simulation is in good agreement with the exact solution, except near the lower boundary, even for the coarsest grid simulation.

Developing Flow in a Channel

The second test problem concerns the development of laminar flow in the entrance of a two-dimensional channel. The problem definition is shown with coarsest CATHENA/PACE-2D simulation grid in Figure 12. The flow field is symmetric about the centreline of the channel so that only the region from the channel wall to the centreline was included in the simulation. The boundary conditions used in simulations were as follows:

1) uniform flow at the inlet boundary,

$u = U$ along $z = 0$,

2) constant pressure at the right-hand boundary,

$P = C$ along $z = 6$,

3) zero flow through the channel centreline,

$v = 0$ along $y = 0.75$, and

4) zero flow through and along the lower boundary,

$u = 0$ and $v = 0$ along $y = 0$.

Again, the constant pressure boundary condition along the $x = 6$ outlet was chosen for convenience. The dynamic pressure variation across the boundary layer, however, is small, since the velocities are small.

The analytical solution for laminar flow in a channel inlet can be obtained by matching an expansion of the flat-plate boundary layer solution in the upstream direction with the deviation from the asymptotic parabolic velocity distribution expressed as a series in the downstream direction. The analytical solution is lengthy and the reader is referred to Schlichting [11] for details.

The CATHENA/PACE-2D simulations were performed with water as the fluid at 20°C and at atmospheric pressure ($\rho \simeq 1000$ kg/m^3). An artificially large dynamic viscosity ($\mu = 0.1$ kg/m•s) was used to make the growth of the boundary layer from the inlet to the asymptotic parabolic velocity distribution clearly visible. The flow boundary condition for the velocity was $U = 1 \times 10^{-2}$ m/s.

Three simulations of the developing flow were performed refining the grid. Grid refinement was only conducted in the cross-stream, direction y. Simulations were conducted with a 7 by 3, a 7 by 9 and a 7 by 15 grid system.

The simulation results for the flow field are compared with the analytical solution in Figures 13 through 15. The vectors in these figures represent the x-component of the velocity in the simulation at the centre-line of each grid location. The analytical solution is represented by the velocity profile at each grid location in the x-direction.

The results demonstrate that the CATHENA/PACE-2D solution is converging towards the analytical solution, with exception of the grid closest to the wall, as the grid is refined. The CATHENA/PACE-2D simulation uses a wall shear formula for the grid adjacent to a wall. These results indicate that the application of the wall shear formula used in the prototype code requires further examination.

8. CONCLUSIONS

The prototype CATHENA/PACE-3D code package represents the first attempt to model, in a fully integrated sense, the thermalhydraulic and aerosol events that could follow a postulated accident in a CANDU reactor. As such, it is the closest we have yet been able to come to producing a tool for best-estimate calculations of the potential "source-term" hazard to the public. Initial code results are very encouraging.

Future work will involve specifying a replacement solution procedure for the basic set of linear equation (the sparse-matrix solver used in CATHENA cannot easily cope with the non-sparse structure encountered with large three-dimensional systems) and further examination of the wall shear formulation. In due course, the models described here will be further refined and coupled to models for fuel, fuel channel and hydrogen behaviour for improved analysis of postulated severe-fuel-damage reactor accidents.

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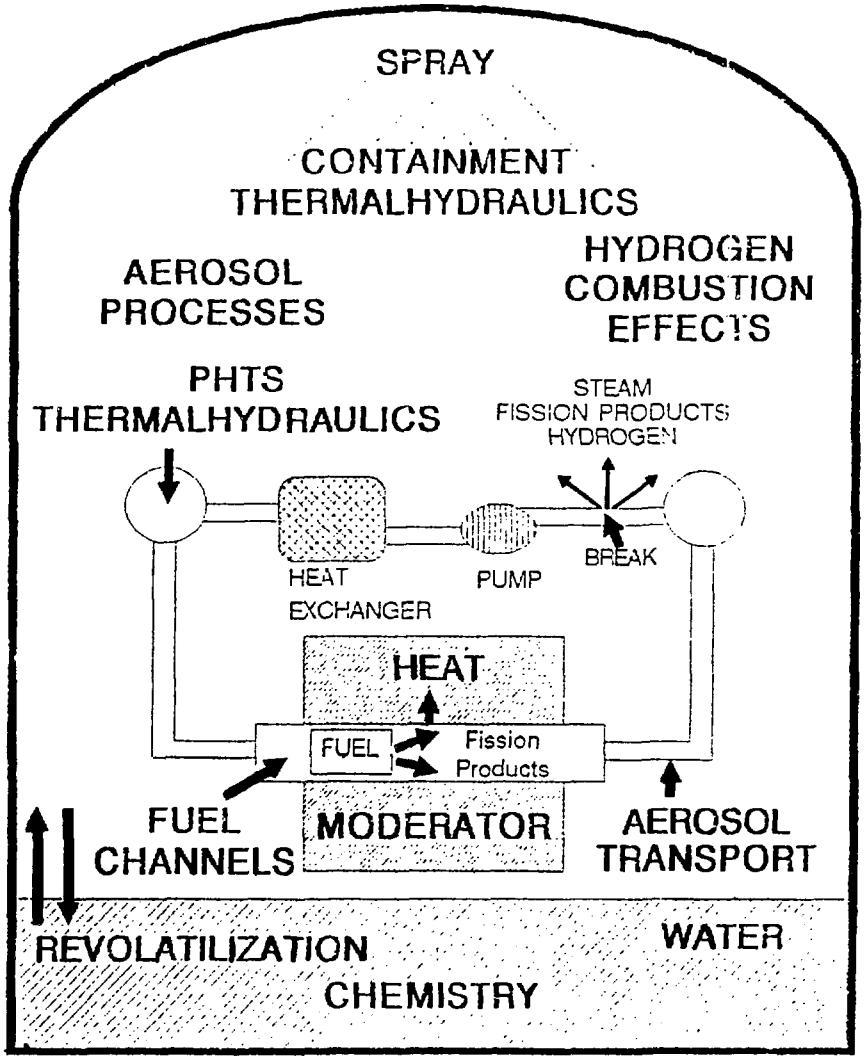

FIGURE 1: Reactor Accident Phenomena

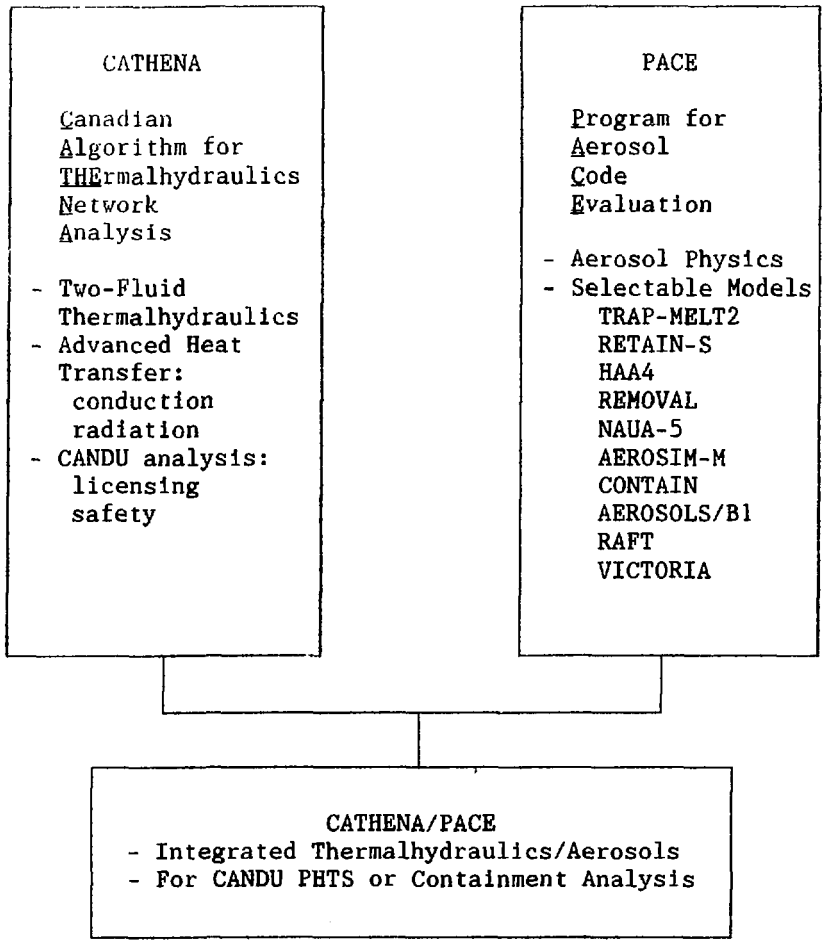

FIGURE 2: The Integrated CATHENA/PACE Code for Coupled Thermalhydraulics and Aerosol Physics Analysis

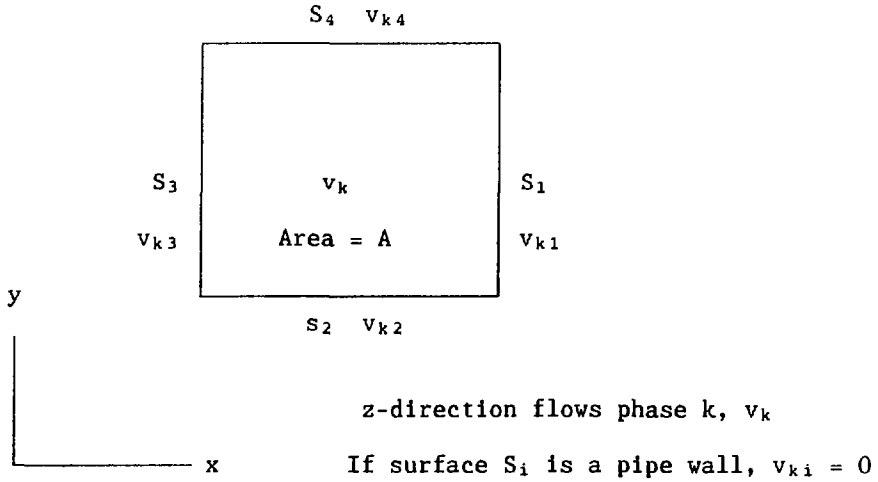

FIGURE 3: Typical Adjacent Flow Structure for CATHENA/PACE-3D Analysis

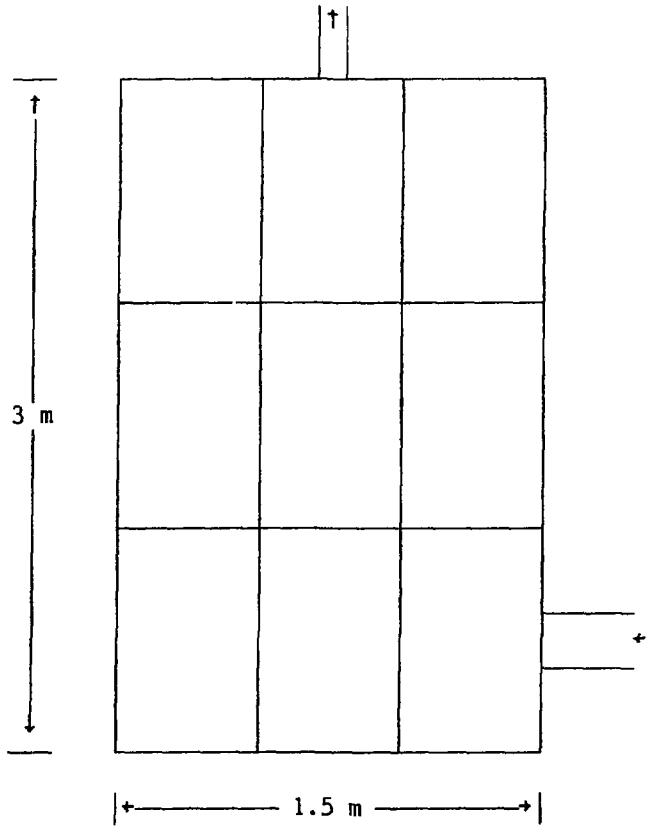

FIGURE 4: An Example 3-D Test Tank

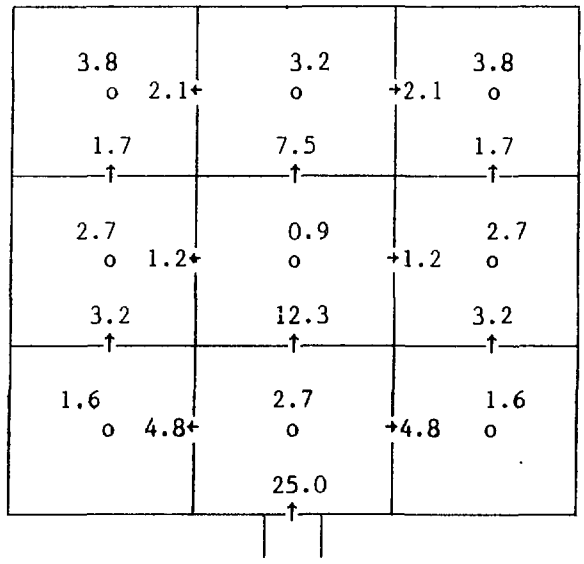

FIGURE 5: CATHENA/PACE-3D Results: Flows in the Bottom Slice of the 3-D Test Tank

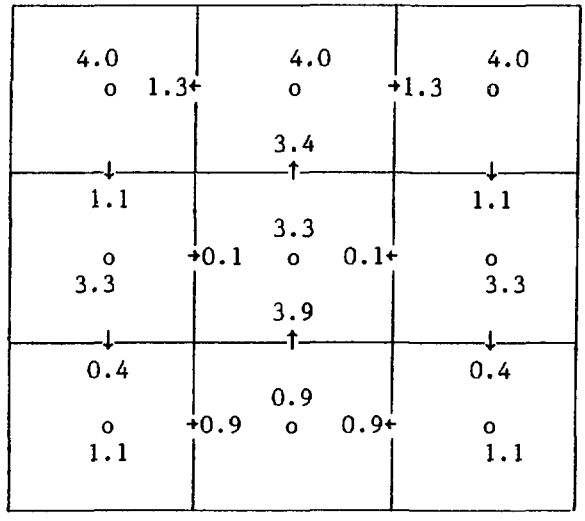

FIGURE 6: CATHENA/PACE-3D Results: Flows in the Middle Slice of the 3-D Test Tank

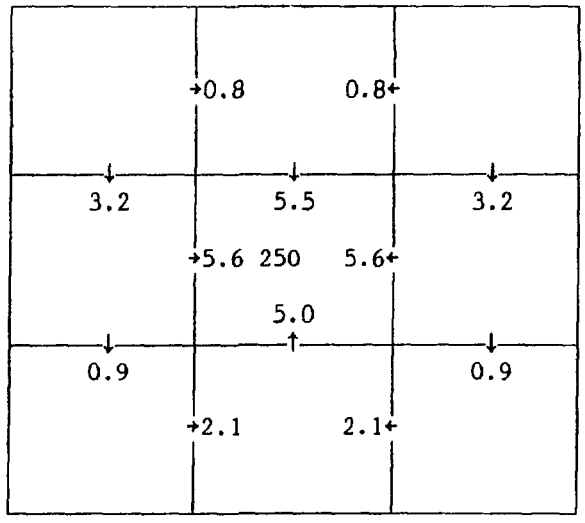

FIGURE 7: CATHENA/PACE-3D Results: Flows in the Top Slice of the 3-D Test Tank

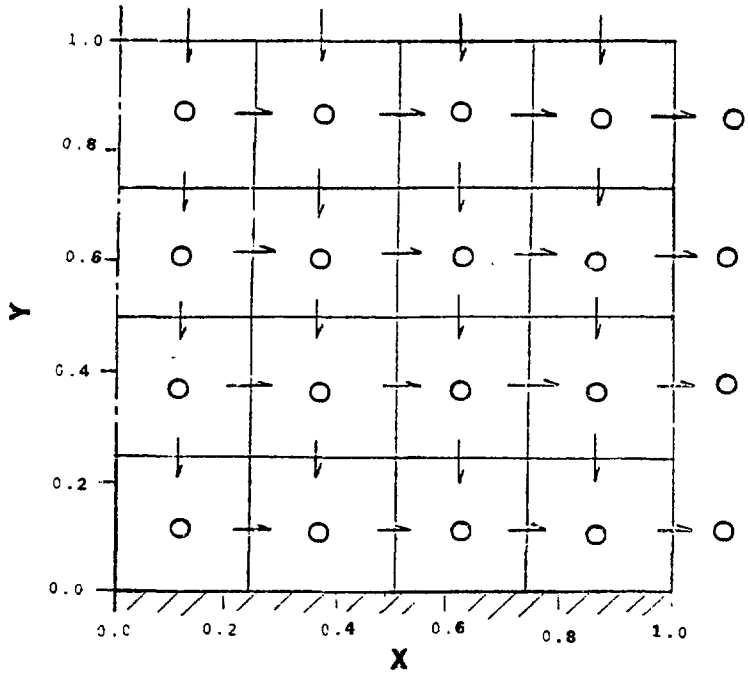

FIGURE 8: Flow into a Stagnation Point: Test Problem Definition

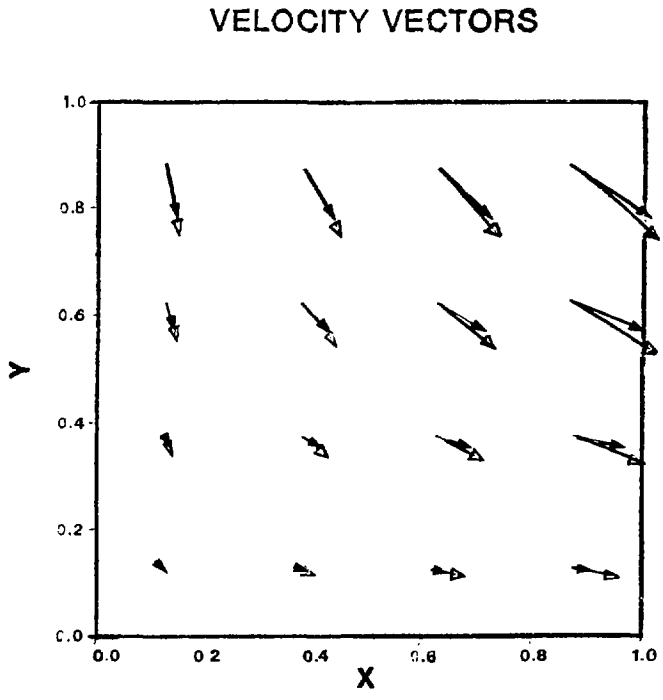

FIGURE 9: Flow into a Stagnation Point: CATHENA/PACE-2D Results with a 4 by 4 Grid. (The solid arrowhead is the analytical solution.)

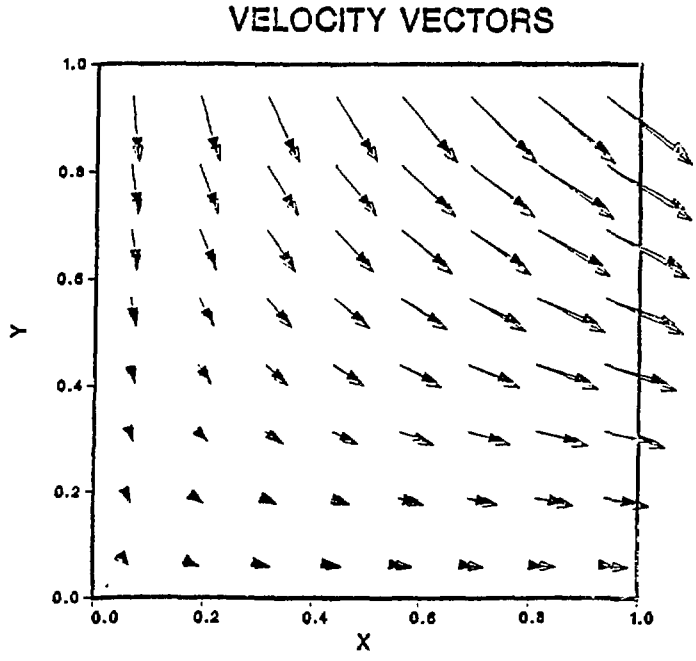

FIGURE 10: Flow into a Stagnation Point: CATHENA/PACE-2D Results with a 8 by 8 Grid. (The solid arrowhead is the analytical solution.)

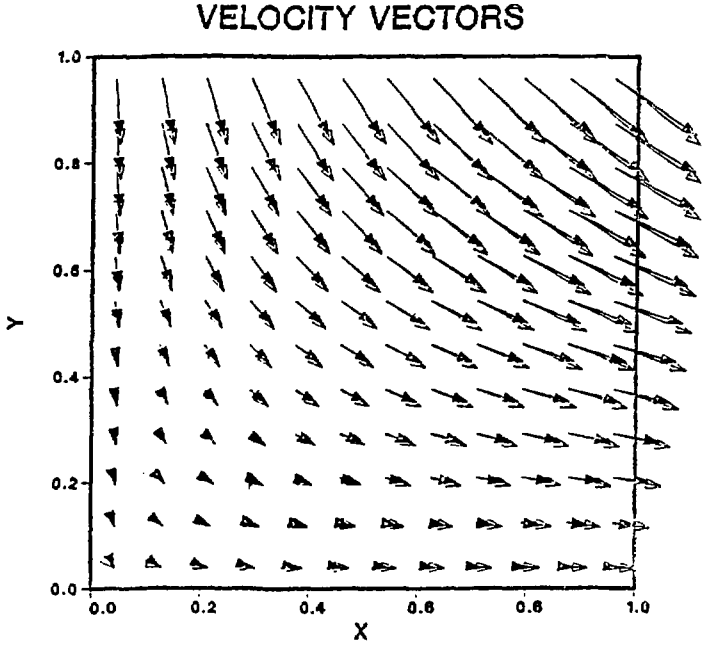

FIGURE 11: Flow into a Stagnation Point: CATHENA/PACE-2D Results with a 12 by 12 Grid. (The solid arrowhead is the analytical solution.)

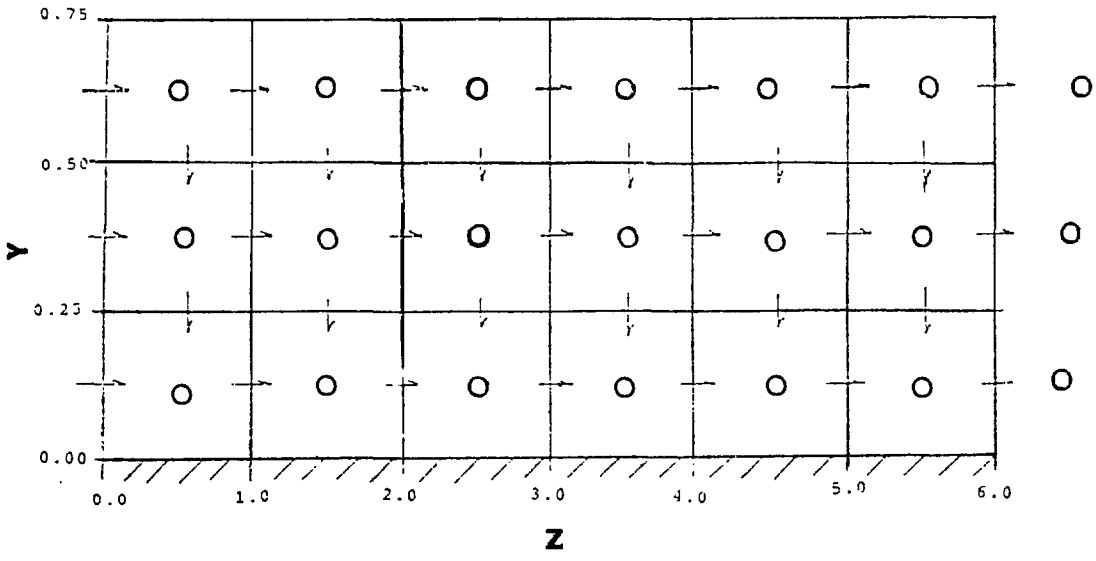

FIGURE 12: Developing Flow in a Channel: Test Problem Definition

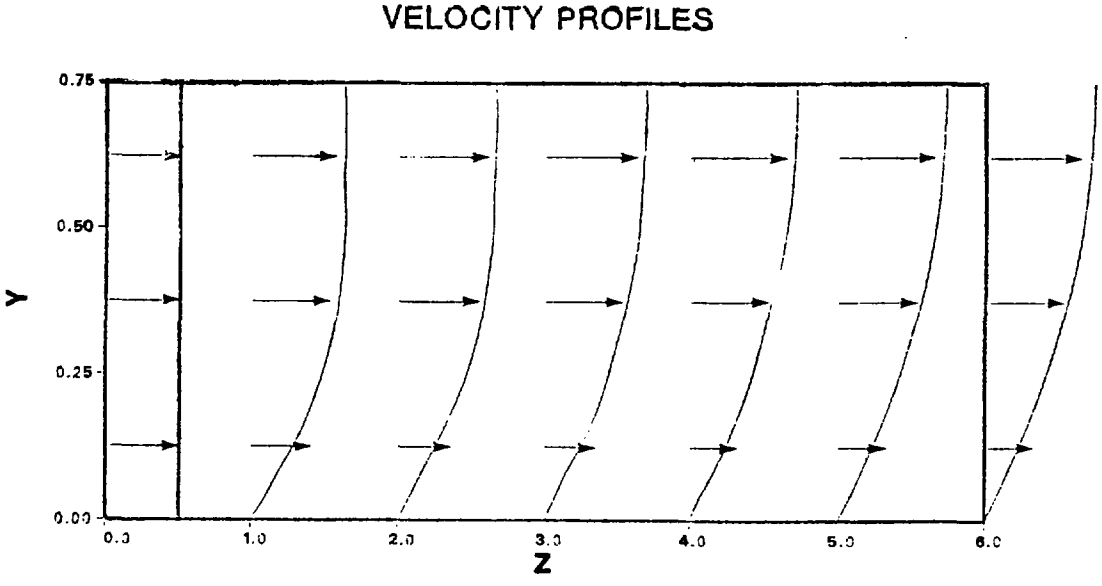

FIGURE 13: Developing Flow in a Channel: CATHENA/PACE-2D Results with a 7 by 3 Grid

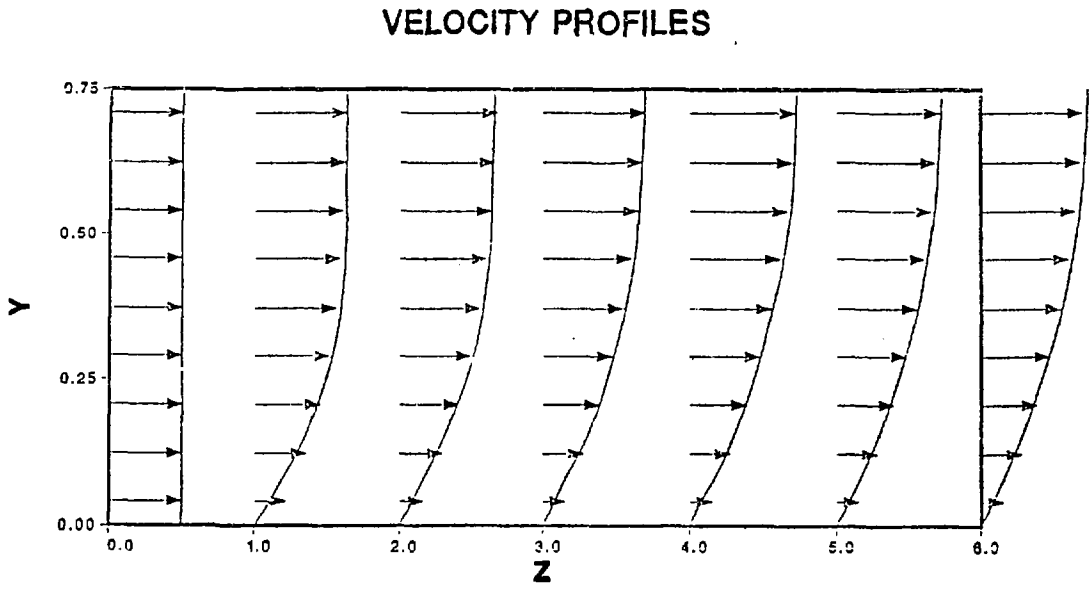

FIGURE 14: Developing Flow in a Channel: CATHENA/PACE-2D Results with a 7 by 9 Grid

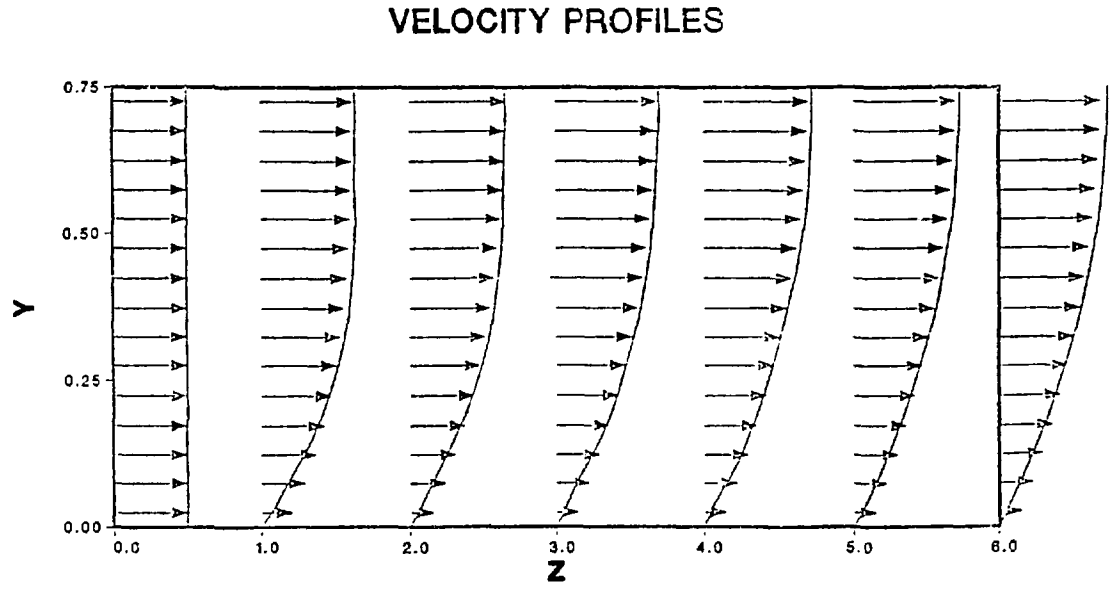

FIGURE 15: Developing Flow in a Channel: CATHENA/PACE-2D Results with a 7 by 15 Grid

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