MIXING OF BUOYANT COMBUSTIBLE GASES
IN BWR CONTAINMENT SYSTEMS

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By

D. S. Trent

August 1973

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TABLE OF CONTENTS

	<u>Page</u>
INTRODUCTION	1
SUMMARY.	5
THEORETICAL DEVELOPMENT.	7
Governing Equations	7
Conservation of Energy.	12
Auxiliary Thermodynamic Relationships	14
COMPUTER PROGRAM	16
Computer Input/Output	16
TEST RESULTS	18
REFERENCES	22

FIGURES

<u>Figure No.</u>		<u>Page</u>
1.	GE MARK-I and MARK-III BWR Containment Systems	2
2.	Cross-Section of BWR MARK-I Pressure Suppression Chamber (Torus)	8
3.	Rectangular Torus for Code Testing (Test Case 1)	19
4.	Streamlines for Pressure Suppression Chamber (Test Case 1)	20
5.	Isotherms for Pressure Suppression Chamber (Test Case 1)	21
6.	Radial Velocity Profiles for Test Case 1	22
7.	Vertical Velocity Profiles for Test Case 1	23

MIXING OF BUOYANT COMBUSTIBLE GASES
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D. S. Trent

INTRODUCTION

Following a loss of coolant accident in a BWR system, hydrogen gas may accumulate within the containment vessel as a result of:

- metal-water reaction involving the zirconium fuel cladding and reactor coolant, and
- long term radiolytic decomposition of the emergency coolant.

If a sufficient amount of hydrogen is generated, it may react with the oxygen present in the containment atmosphere at a rate sufficiently rapid to result in significant overpressurization of the containment vessel.

As part of the safety analysis report, a license applicant must provide calculations which indicate the rate of hydrogen generation from each of these potential sources and show that provisions have been made to maintain the concentration of hydrogen below its lower flammable limit. Safety guide 7 provides the regulatory position on the assumptions to be made in these calculations. Careful independent evaluation of the information supplied by the applicant is necessary to assure that all possibilities for developing flammable mixtures have been considered and ruled out as being not credible. Since the density of hydrogen is markedly different from the other constituents of the containment atmosphere, the potential for stratification and pocketing of significant concentrations of hydrogen must be recognized.

Figure 1 illustrates schematic diagrams of the GE MARK-I and MARK-III BWR/6 containment systems. Following LOCA in either of these systems, the initial transient would produce hydrogen by metal-

FIGURE 1. GE MARK-I and MARK-III BWR Containment Systems.

water reaction with the zirconium clad fuel. Simultaneously, large quantities of steam would be produced within the core and ejected to the drywell through the postulated coolant system break. This sequence of events pressurizes the drywell with LOCA steam which is then forced to the pressure suppression chamber and condenses within the suppression pool.

In the BWR pressure suppression chamber the danger from stratification is associated with the radiolytic generation of both hydrogen and oxygen. Within the suppression chamber radiolysis generates a 2:1 mixture of hydrogen:oxygen which is released to the N_2 atmosphere at the liquid-gas interface. Since this process continues for a matter of months, explosive concentrations of H_2/O_2 can occur within the containment system unless Containment Atmosphere Dilution (CAD) is used. CAD is a process whereby N_2 is added to the system to insure that the gross concentration of H_2/O_2 is maintained below a combustible level. However, CAD does not insure that local concentrations will not build up to explosive levels as a result of poor local mixing. During CAD the pressure within the pressure suppression chamber will increase as a function of N_2 addition and radiolytic generation of H_2/O_2 , and the containment pressure will eventually equilibrate through leakage. Until pressure equilibration is reached mass accumulation occurs at a very slow rate within the chamber.

Because the calculations required for predicting hydrogen stratification under the anticipated conditions are very complex, assessments are generally presented by applicants in a rather approximate manner or treated somewhat subjectively. A more quantitative method of evaluating the potential for significant stratification of hydrogen in the presence of diffusion, natural convection, and turbulent mixing would provide a more reliable assessment of requirements for assuring

hydrogen stratification will not occur.

Analysis concerning the extent of natural circulation and mixing are to be conducted by numerical computation using the COVEC computer code developed in this study. Since there is mass accumulation during pressurization (CAD) computing the natural convection and mixing is a time dependent problem. However, the characteristic time scale of the convective motion is smaller than that of the mass accumulation (seconds vs. months). Hence, it would be imprudent to use a true transient approach for solving the governing equations since the time steps would need to be on the order of second and simulation of conditions over durations of interest (months) would require an unreasonable amount of computer time. To alleviate this problem a psuedo-transient approach is taken whereby it is assumed that time dependent quantities in the governing equations are known in terms of boundary and local steady flow conditions. To carry out this approach the COVEC code was modified to accommodate accumulation of mass species (N_2 and H_2/O_2). In this manner equilibrium convection currents and H_2/O_2 concentrations are computed based on a constant pressurization rate and constant generation of radiolytic H_2/O_2 .

SUMMARY

The computer code SYMJET,⁽¹⁾ initially developed to calculate turbulent mixing in buoyant plumes, has the capability of calculating recirculating flow fields in the presence of heat and mass transport. This code has been modified to compute convection currents and concentration distributions of hydrogen/oxygen (stratification) in the pressure suppression chamber of a BWR following LOCA. The first modified version of SYMJET called COVEC (Code for Vorticity-Energy Convection) solves the partial differential equations which govern momentum, energy and mass transport in closed or open axisymmetric heat transfer systems without mass accumulation. Although COVEC can handle only axisymmetric containment configurations, programming has been carried out so that any axisymmetric shape may be specified by input. Hence, steady flow analysis of liquid or gas phases can be readily performed on any of the containment systems where axisymmetric approximations are valid (i.e., BWR drywell, BWR pressure suppression chamber, PWR containment).

To accommodate mass accumulation during CAD and radiolysis, the COVECA code is presently being developed. This code solves the governing equations on a pseudo-time dependent basis where mass accumulation and pressurization are prescribed functions of time. This approach is possible since the time scale for accumulation is much larger than the time scale for convection currents. The status of code development is as follows:

- The COVEC code has been programmed, tested and converted from the UNIVAC 1108 to the CDC 6600 CYBER 74 (no accumulation).
- The COVECA code has been developed and tested on the CYBER 74 for a case without mass accumulation.

- Portions of the COVECA code which deal with accumulation are in the debug stage at this writing.

The finished version of COVECA will simulate convection currents and mixing for any axisymmetric geometry and will have capabilities to handle the following conditions:

- natural and/or forced convection,
- buoyancy a function of temperature, pressure and constituent types,
- transport of up to 3 individual constituents,
- slow accumulation (pressurization) of containment space,
- simultaneous heat transfer in containment solid walls,
- internal generation of heat or constituents.

Output for the computer program will include

- point-wise velocity field,
circulation patterns in containment space,
- point-wise temperature field,
point-wise concentration distribution of each mass species (N_2 and H_2/O_2).

THEORETICAL DEVELOPMENT

Consider the steady flow of mass species m_i (N_2) to a two-dimensional axisymmetric vessel which is otherwise impervious to mass flow (Figure 2). We permit pressurization of the vessel at a very slow rate by virtue of the flow $\dot{m}_i$ and also by evolution of other mass species $\dot{M}_j$ (H_2, O_2). It is assumed that the very slow flow rate of $\dot{m}_i$ occurs from a source at a much greater pressure than the pressure within the vessel so that $\dot{m}_i$ is steady in time or at least is not directly influenced by the vessel pressure.

Assumptions are:

- $\dot{m}_i$ and $\dot{M}_j$ are known functions of time.
- $\bar{P}$, the vessel thermodynamic pressure, is large compared to spatial pressure gradients such as those that promote natural circulation.
- Likewise, the density at any point within the vessel is assumed to be large compared to spatial changes of density (i.e., $|\Delta\rho/\rho| \lll 1$, Boussinesq approximation).
- Boundary conditions for heat transfer may be given in terms of a known temperature or flux and are steady.
- Constituent concentration boundary conditions or generation rates are known and steady.
- The boundary flow of volume is slow compared to the total volume.

Governing Equations

For the case at hand we are concerned about long term transient behavior (order of months). The problem involves mass accumulation which occurs at a very slow rate, hence has a large time scale. Com-

FIGURE 2. Cross-Section of BWR MARK-I Pressure Suppression Chamber (Torus).

pared to the mass accumulation, the time scale for natural circulation is very small, hence it is unwise to approach the problem solution from true transient analysis since very large and prohibitive amounts of computer time would be required.

The approach taken here is based on psuedo-steady approximations whereby the transient part of the problem (mass accumulations and pressurization) is assumed to be a known function of time based on thermodynamic principles alone.

Continuity:

$$\frac{\partial \rho^*}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r \rho^* u) + \frac{\partial}{\partial z} (\rho^* v) = 0 \quad (1)$$

where ρ^* is the total density of the mixture at a point in the vessel and can be calculated by an appropriate thermodynamic equation of state.

According to our assumptions concerning continuity, spatial changes of density can be ignored since they will be very small, that is,

$$u \frac{\partial \rho^*}{\partial r} \approx v \frac{\partial \rho^*}{\partial z} \approx 0 \quad (2)$$

However, the term involving time change of density cannot be ignored since it is the quantity that accounts for accumulation. Hence, the continuity equation may be written as

$$\frac{1}{r} \frac{\partial u r}{\partial r} + \frac{\partial v}{\partial z} = - \frac{1}{\rho^*} \frac{\partial \rho^*}{\partial t} \quad (3)$$

Pressure gradients within the vessel will be small compared to the over pressure which implies that pressure at any point may

be established by the gas law

$$\bar{P} = \bar{\rho}^* \bar{R}^* \bar{T} \quad (4)$$

where R^* is the gas constant for the mixture and the overbars denote average quantities. Hence to an approximation satisfactory for continuity, the right hand side of Equation (3) may be replaced as follows:

$$-\frac{1}{\bar{\rho}^*} \frac{\partial \bar{\rho}^*}{\partial t} = -\frac{1}{\bar{P}} \frac{\partial \bar{P}}{\partial t} = -\frac{1}{\bar{P}} \frac{\Delta \bar{P}}{\Delta t} \quad (5)$$

Momentum:

The governing equations for momentum transport in axisymmetric coordinates are given by:

r - direction

$$\frac{Du}{Dt} = -\frac{\partial p^0}{\partial r} + \frac{\partial}{\partial r} \left(\frac{\epsilon_r}{r} \frac{\partial u}{\partial r} r \right) + \frac{\partial}{\partial z} \left(\epsilon_z \frac{\partial u}{\partial z} \right) \quad (6)$$

z - direction

$$\frac{Dv}{Dt} = -\frac{\partial p^0}{\partial z} + B + \frac{1}{r} \frac{\partial}{\partial r} \left(r \epsilon_r \frac{\partial v}{\partial r} \right) + \frac{\partial}{\partial z} \left(\epsilon_z \frac{\partial v}{\partial z} \right) \quad (7)$$

where the symbols are defined below.

u = radial velocity component

v = axial velocity component

ϵ_r = radial component of eddy momentum diffusivity

ϵ_z = vertical component of eddy momentum diffusivity

$B = \frac{g}{\rho_r} (\rho_r - \rho)$ (from Boussinesq approximation)

p^0 = deviatoric pressure

ρ_r = reference density

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial r} + v \frac{\partial}{\partial z}$$

Fluid vorticity may be defined by

$$\omega = \frac{\partial u}{\partial z} - \frac{\partial v}{\partial r} \quad (8)$$

A stream function ψ and scalar potential ϕ are defined by:

$$u = -\frac{1}{r} \frac{\partial \psi}{\partial z} + \frac{\partial \phi}{\partial r} \quad (9)$$

and

$$v = \frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{\partial \phi}{\partial z} \quad (10)$$

Substituting Equations (9) and (10) into Equation (8) yields

$$\frac{\partial^2 \psi}{\partial r^2} - \frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial z^2} = -r\omega \quad (11)$$

Substituting Equations (9) and (10) into the continuity

Equation (3) yields

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial z^2} = -\frac{1}{\rho^*} \frac{\partial \rho^*}{\partial t} \quad (12)$$

Hence, the velocity distributions in the vessel may be solved for by using Equations (9) and (10) once the values of ψ and ϕ are resolved from Equations (11) and (12), respectively, Equation (12) may be solved once the value of $\frac{1}{\rho^*} \frac{\partial \rho^*}{\partial t}$ is established, but Equation (11) requires the vorticity distribution, ω .

A transport equation for ω may be obtained by cross-differentiating Equations (6) and (7) followed by subtraction of the latter result from the former. This operation leads to

$$\frac{\partial \omega}{\partial t} + \left(\frac{1}{r} \frac{\partial u r}{\partial r} + \frac{\partial v}{\partial z} \right) \omega + \frac{\partial u}{\partial r} \omega + \frac{\partial v}{\partial z} \omega = - \frac{\partial B}{\partial r} + \epsilon_r \frac{\partial}{\partial r} \left[\frac{1}{r} \frac{\partial \omega r}{\partial r} \right] + \epsilon_z \frac{\partial^2 \omega}{\partial z^2} \quad (13)$$

or for constant eddy transport coefficients

$$\frac{D\omega}{Dt} - \frac{1}{\rho} \frac{\partial \rho^*}{\partial t} \omega = - \frac{\partial B}{\partial r} + \epsilon_o \left\{ \frac{\partial}{\partial r} \left[\frac{1}{r} \frac{\partial \omega r}{\partial r} \right] + \frac{\partial^2 \omega}{\partial z^2} \right\} \quad (14)$$

Conservation of Energy

The energy equation is

$$\begin{aligned} & \frac{\partial \rho^* (e + P/\rho^*)}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} [r \rho^* u (e + P/\rho^*)] \\ & + \frac{\partial}{\partial z} [v \rho^* (e + P/\rho^*)] + \dot{Q} = \frac{1}{r} \frac{\partial}{\partial r} \left(r k_r \frac{\partial T}{\partial r} \right) + \frac{d}{dz} \left(k_z \frac{\partial T}{\partial z} \right) \end{aligned} \quad (15)$$

where $e = u^* + \frac{\bar{v}^2}{2} + gz$.

Since the two mechanical energy terms are small compared to the mixture internal energy, u^* , we let

$$e = u^*.$$

The perfect gas law is a good approximation for the thermodynamic condition of the vessel atmosphere, hence

$$u^* = C_v^* T$$

and

$$C_p^* T = C_v^* T + P/\rho^* = h \text{ (enthalpy)} \quad (16)$$

The symbols C_p^* and C_v^* are the mixture specific heats at constant pressure and constant volume, respectively. Eliminating spatial and time changes of C_p^* , the energy equation may be expressed as

$$\frac{\partial \rho^* T}{\partial t} - \frac{1}{C_p^*} \frac{\partial P}{\partial t} + \frac{1}{r} \frac{\partial r u \rho^* T}{\partial r} + \frac{\partial v \rho^* T}{\partial z} + \frac{\dot{Q}}{C_p^*} =$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\rho^* \epsilon_{Hr} r \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(\rho^* \epsilon_{Hz} \frac{\partial T}{\partial z} \right) \quad (17)$$

From the perfect gas law

$$\frac{\partial \rho^* T}{\partial t} = \frac{1}{R^*} \frac{\partial P}{\partial t} \quad (18)$$

where R^* is the mixture gas constant.

Since density gradients will be small, we may eliminate spatial changes of ρ^* in dealing with energy conservation but must include $\partial \rho^* T / \partial t$ since this term represents energy accumulation.

Therefore,

$$\frac{1}{\rho^*} \left[\frac{1}{R^*} - \frac{1}{C_p^*} \right] \frac{\partial P}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r u T) + \frac{\partial}{\partial z} (v T) + \frac{\dot{Q}}{\rho^* C_p^*} =$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\epsilon_{Hr} r \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(\epsilon_{Hz} \frac{\partial T}{\partial z} \right) \quad (19)$$

The term

$$\frac{1}{\rho^*} \left[\frac{1}{R^*} - \frac{1}{C_p^*} \right] \approx \frac{-1}{\rho^* C_p^*} \quad (20)$$

since

$$\frac{1}{R^*} \ll \frac{1}{C_p^*} \quad (21)$$

Transport of Constituents O_2 , H_2 and N_2

The mass fraction of constituent i is defined as

$$f^i = \frac{M^i}{M_t} = \frac{\rho^i}{\rho^*} \quad (22)$$

The transport equation for species i is

$$\begin{aligned} \frac{\partial f^i \rho^*}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} [r u f^i \rho^*] + \frac{\partial}{\partial z} [v f^i \rho^*] + \dot{m}_i = \\ \frac{1}{r} \frac{\partial}{\partial r} [r \epsilon_{ir} \frac{\partial f^i \rho^*}{\partial r}] + \frac{\partial}{\partial z} [\epsilon_{iz} \frac{\partial f^i \rho^*}{\partial z}] \end{aligned} \quad (23)$$

Noting again that spatial gradients of density are small for the system which we are considering, ρ^* may be extracted from the gradient terms so that Equation (23) becomes

$$\begin{aligned} \frac{1}{\rho^*} \frac{\partial f^i \rho^*}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} [r u f^i] + \frac{\partial}{\partial z} [v f^i] + \frac{\dot{m}_i}{\rho^*} = \\ \frac{1}{r} \frac{\partial}{\partial r} [r \epsilon_{ir} \frac{\partial f^i}{\partial r}] + \frac{\partial}{\partial z} [\epsilon_{iz} \frac{\partial f^i}{\partial z}] \end{aligned} \quad (24)$$

Now,

$$\frac{1}{\rho^*} \frac{\partial f^i \rho^*}{\partial t} = \frac{\partial f^i}{\partial t} + \frac{f^i}{\rho^*} \frac{\partial \rho^*}{\partial t}$$

and since we are dealing with a solution which is steady in time

$$\frac{\partial f^i}{\partial t} \equiv 0.$$

Auxiliary Thermodynamic Relationships

The following relationships are based on the Gibbs-Dalton law for mixture of idea gases where N is the total number of constituents.

$$\rho^* = \sum_i^N \rho^i f^i \quad (25)$$

$$R^* = \sum_i^N R^i f^i \quad (26)$$

$$c_p^* = \sum_i^N c_p^i f^i \quad (27)$$

$$\bar{p} = \sum_i^N p^i \quad (28)$$

$$1 = \sum_i^N f^i \quad (29)$$

In Equation (28) above, p^i is the partial pressure of the i th gas species.

COMPUTER PROGRAM

The computer program being developed to calculate natural circulation and constituent concentration in the BWR pressure suppression chamber is an extension of the COVEC code which solves Equations (11), (14) and (19) with the time dependent terms set to zero. The modified version of COVEC (COVECA) necessary for the present work involves retaining the pseudo-time dependent terms in order to account for mass and energy accumulation.

Required equations are as follows:

Equation (11)	-	ψ
Equation (12)	-	ϕ
Equations (9) & (10)	-	u and v
Equation (14)	-	ω
Equation (19)	-	T
Equation (24)	-	f^i (N-1 equations needed where i = 1, 2, ..., N)

Computer Input/Output

Input

1. Geometry (code will accommodate any axisymmetric geometry)
2. Boundary conditions
 - thermal
 - flow
 - constituents
3. Generation rates

- heat

- mass species

4. Physical properties

5. Stationary conditions

- total mass

- total pressure

Output

- point-wise velocity field

- circulation patterns

- point-wise temperature field

- point-wise concentration distribution of each mass

species (N_2 , H_2/O_2)

TEST RESULTS

Initial testing of the COVEC and COVECA codes was carried out for a torus chamber having rectangular cross-section as shown in Figure 3 (Test Case 1). This test problem has no mass accumulation or boundary mass flow and convective currents are driven entirely by the temperature difference between the chamber walls and suppression pool. The test problem has been run successfully on both the UNIVAC 1108 and the CDC 6600, CYBER 74. The version of COVECA tested has the capability to accommodate mass accumulation but this option of the program is still in the debug stage and was not tested.

Results of the COVECA test runs are shown in Figures 4 through 7. Figure 4 illustrates the convections pattern that can be expected driven by heat transfer alone. The thermal distributions are shown by Figure 5. Figures 6 and 7 show the chamber radial and vertical velocity profiles, respectively. As the illustrations indicate, two large cells are set up which rotate slowly counter to one another. The dividing streamline is displaced radially from center because the section of the torus represents a truncated pie-shaped radial slice where the left wall is 40 feet and the right or outer wall is 72 feet from the containment system centerline.

Future testing of the COVECA code will follow three steps:

- simulation of the Figure 3 geometry and thermal boundary conditions with CAD (N_2 pressurization),

FIGURE 3. Rectangular Torus for Code Testing (Test Case 1).

FIGURE 4. Streamlines for Pressure Suppression Chamber (Test Case 1).

$D_0 = 16$ feet

FIGURE 5. Isotherms for Pressure Suppression Chamber (Test Case 1).

FIGURE 6. Radial Velocity Profiles for Test Case 1.

FIGURE 7. Vertical Velocity Profiles for Test Case 1.

- simulation of the system without CAD but with H_2/O_2 radiolytic generation,
- simulation of the system with both CAD and H_2/O_2 generation.

During the same period, code proof testing will be carried out for laminar flow in a vertical cylinder without mass accumulation. Code results will be tested against a numerical solution and experimental data published in the literature for a case of bottom heating and side wall cooling (or vice versa). Once the proof testing and accumulation tests have been completed, the COVECA code will be considered operational.

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