EG&G Idaho, Inc.

WR-CD-81-055 PDR

December 1981

NRC Research and/or Technical Assistance Report

INTERNAL TECHNICAL REPORT

TRAC-BWR COMPLETION REPORT
CORRECTION TO METAL-WATER REACTION MODEL

CODE DEVELOPMENT DIVISION

M. M. Giles

Walter L Weaver III

EG&G Idaho, Inc

FORM EG&G-398
(Rev. 11-81)

INTERIM REPORT

Accession No. __________

Report No. WR-CD-81-055

Contract Program or Project Title: Loss-of-Coolant Accident Analysis Development

Subject of this Document: TRAC-BWR Completion Report
Correction to Metal-Water Reaction Model

Type of Document: Technical Report

Author(s): M. M. Giles

Date of Document: December 1981

Responsible NRC/DOE Individual and NRC/DOE Office or Division: F. Odar, NRC-RES

> This document was prepared primarily for preliminary or internal use. It has not received full review and approval. Since there may be substantive changes, this document should not be considered final.

EG&G Idaho, Inc.
Idaho Falls, Idaho **83415**

Prepared for the
U.S. Nuclear Regulatory Commission
Washington, D.C.
Under DOE Contract No. **DE-AC07-76ID01570**
NRC FIN No. A6052

INTERIM REPORT

WR-CD-81-055

December 1981

TRAC-BWR COMPLETION REPORT

CORRECTION TO METAL-WATER REACTION MODEL

M. M. Giles

Approved

Walter L. Weaver III

Walter L. Weaver, III
Acting Section Supervisor
TRAC-BWR Section

CONTENTS

CORRECTION TO METAL-WATER REACTION MODEL

1. INTRODUCTION

The existing metal-water reaction model in TRAC-BD1 has been found deficient in that the volume of reacted zircaloy metal is overestimated by about 50%. This results in a corresponding overestimation of the metal-water reaction heat source, resulting in anomalously high fuel rod temperatures under certain conditions. The metal volume overestimation results because of the implicit assumption that the volume of a given mass of zircaloy metal is the same as the volume of zirconium oxide formed when that mass of metal is totally oxidized. In fact, a volume increase of about 50% occurs during the oxidation process.

This deficiency has been noted by the Los Alamos National Laboratory TRAC group and has been corrected in TRAC-PD2. The correction is achieved by using a reaction rate equation based on weight of oxygen consumed rather than on rate of change of oxide layer thickness as used in TRAC-P1A and TRAC-BD1. The new method removes an inherent difficulty in relating oxide layer thickness to volume of reacted metal. The new model is functionally identical to the old model, the only practical difference being in the choice of constants used in the two models.

This update serves to implement the TRAC-PD2 metal-water reaction model into TRAC-BD1.

An additional deficiency is corrected by this update set. In the TRAC-P1A model when the oxide thickness exceeds the cladding thickness, the metal-water reaction calculation is bypassed, but the metal-water reaction heat source QWRX retains the value that it had during the time step which consumed the final remaining zircaloy in the cladding. Thus, an erroneous metal-water reaction heat flux remains even though the reaction is no longer occurring. This update set defines QWRX to be zero when the inner radius of the oxidized region is less than or equal to the inner radius of the cladding.

2. MATHEMATICAL MODEL

Given sufficient steam, the following metal-water reaction rate equation has been found to be valid[1,2]

$$\tau \frac{d\tau}{dt} = Ae^{-B/T} \qquad (1)$$

where

τ = total oxygen consumed (kg/m^2)

A = 16.8 kg^2/m^4s

B = 20070 K.

The kinetic parameter τ may be related to the radius of the reacting surface by the relationship

$$1.5\,(R_o - r) = \frac{\tau}{0.26\ \rho_{ZrO_2}} \qquad (2)$$

where

r = reacting surface radius

R_o = original outer radius of cladding

ρ_{ZrO_2} = density of zirconium oxide

0.26 is the weight fraction of oxygen in ZrO_2.

Equation (2) is based on a reacted material volume expansion of 50%, consistent with a density ratio ρ_{ZrO_2}/ρ_{Zr} = 0.90. Eliminating τ from Equations (1) and (2) we obtain

$$-\frac{dr}{dt} = \frac{A}{C(R_o - r)}\, e^{-B/T} \qquad (3)$$

where $C = (0.351\ \rho_{Zr})^2 = 5.22E6\ kg^2/m^6$, using $\rho_{Zr} = 6510\ kg/m^3$.

The method outlined in Reference 1 is used to calculate the zirconium-oxide penetration depth and associated heat source. The mass per unit length of zirconium (m'_{Zr}) consumed by the reaction in one time step is

$$m'_{Zr} = \pi \rho_{Zr} \left[(r^n)^2 - (r^{n+1})^2 \right] \quad (4)$$

Equation (3) is used to calculate r^{n+1}, yielding

$$r^{n+1} = R_o - \left[(r^n)^2 + 2 \frac{A}{C} \Delta t \exp\left(-\frac{B}{T}\right) \right]^{1/2} \quad (5)$$

Assuming a one-region clad, the heat source ($\dot{q}'''_{mw}$) added to the conduction equations is

$$\dot{q}'''_{mw} = 6.45 \times 10^6\ m'_{Zr}\ \ \Delta t\ (R_o^2 - R_i^2)\ \pi]^{-1} \quad (6)$$

where R_i is the inner clad radius, and 6.45×10^6 J/kg corresponds to the energy released per kilogram of oxidized zirconium.

3. IMPLEMENTATION INTO TRAC-BD1

The mathematical forms of Equations (4), (5) and (6) are identical to the equations already coded in the existing TRAC-BD1 subroutine MWRX. Only the constants found in these equations differ from the existing TRAC-BD1 model; hence, the implementation of the new model reqires only that a single data statement be changed in subroutine MWRX to implement the constants for the new model. The old and new constants are shown in the table below.

Constant Name	Description	Old Value	New Value
CWR1	2A/C (Eq 5)	2.252E-6	6.434E-6
CWR2	B (Eq 5)	- 18062.0	- 20070.0
CWR3	Heat of reaction	6.513E6	6.45E6

4. REFERENCES

1. J. V. Cathcart, Quarterly Progress Report on the Zirconium Metal-Water Oxidation Kinetics Program, Oak Ridge National Laboratory Report ORNL/NUREG/TM-4[illegible], August 1976.

2. MATPRO - Version 11: A Handbook of Materials Properties for Use in the Analysis of Light Water Reactor Fuel Rod Behavior, Idaho National Engineering Laboratory Report NUREG/CR-0497 TREE-1280, February 1979.