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Mr. Bernard F. Saffell, Jr.
Program Manager
505 King Avenue
Columbus, OH 43201

Dear Mr. Saffell:

Subject: Aerosol Groupings for In-Vessel and Containment Aerosol Codes

In the past, the grouping of chemical elements for calculations of off-site consequences of severe reactor accidents has been based on the groups chosen for the Reactor Safety Study (RSS, WASH-1400). With the advent of the source term analytical procedure as used in BMI-2104, much more information is available on chemical behavior, and chemical elements that were perceived to behave the same in the RSS are now perceived to behave differently. However, the calculations in BMI-2104 did not follow a large number of chemical element groups or chemical compounds and some of the additional insights based on the chemical behavior were lost. Since some of these elements have radionuclides of biological importance (for instance, Np and Pu), the number and grouping of elements followed in the source term calculations has been reviewed for continued adequacy. It has been concluded by consensus among a small group consisting of J. Mitchell, J. Martin, and J. Read of NRC and H. Ludwig of BNL that the grouping should be changed for the Source Term Code Package (STCP). It is expected that future consequence calculations will use the MACCS code, which has no restriction on the number of element groups and would be able to use the expanded information directly. If CRAC or CRAC2 is used, however, the groups may be recombined as necessary to provide the information for the RSS grouping.

The chemical elements, chemical element, groups and chemical compounds followed as aerosols in the analyses for some of the calculations reported in BMI-2104 and the set recommended for the STCP are given in Table 1. For those calculations in BMI-2104 that reported the full Reactor Safety Study release fractions, the grouping of the masses of materials for either in-vessel release or ex-vessel release is given in the first section of Table 1. For those calculations that only reported I, Cs, and Te releases, the grouping of masses is given in the second section of the table. In this latter case, the masses of materials that were previously followed separately were lumped into the aerosol mass.

The justification for the revised set of groups given in the third section of Table 1 can be found in Draft NUREG-0956. Tables 4.8 and 4.9 show higher fractional releases for Ba than Sr for in-vessel releases while Tables 4.10 and 4.11 show the reverse for ex-vessel releases. Therefore, their release fractions could show sequence specific behavior. La and Ce groups are not evaluated in the CORSOR in-vessel release model, but show different ex-vessel release fractions in Tables 4.10 and 4.11. The other lanthanides and actinides previously in the La group were divided according to whether the

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chemistry of La or of Ce was believed to be more appropriate as a surrogate. Separating in-vessel and ex-vessel lumped aerosols will allow hand calculations of oxidized species for sequences where direct heating of the containment atmosphere is assumed.

In all cases the noble gases Xe and Kr are followed in the MARCH calculation and also were reported for the Reactor Safety Study grouping releases. They should continue to be followed for STCP calculations and reported.

In summary, the revised grouping recommended for the STCP calculations should provide the information that will allow off-site consequence calculations to take the best possible advantage of the developing insights on chemical behavior. This letter confirms our telephone request to J. Gieseke in July 1985.

Sincerely,

Original Signed By

M. Silberberg, Branch Chief
Fuel Systems Research Branch
Division of Accident Evaluation
Office of Nuclear Regulatory Research

Enclosure: Table 1

cc: T. Margulies, NRC
J. Martin, NRC
J. Read, NRC
H. Ludwig, BNL
R. Bari, BNL
T. Pratt, BNL
R. Denning, BCL
P. Cybulskis, BCL
J. Gieseke, BCL
D. Powers, SNL
T. Kress, ORNL

DAE:FSRB
Mitchell:md
11/6/85

DAE:FSRB
Meyer
11/7/85

DAE:FSRB
Silberberg
11/7/85

MD

MS

Table 1: Components followed as aerosols in BMI-2104 calculations
and as recommended for STCP calculations.

1. BMI-2104-RSS groups

I-Br*

Cs-Rb*

Te-Sb-Se

Sr-Ba

Ru-Rh-Pd-Tc-Mo

La-Eu-Pr-Nd-Pm-Sm-Y-Nb-Zr(f.p.)-Ce-Np-Pu

Aerosol

2. BMI-2104-Volatile releases only

I-Br*

Cs-Rb*

Te-Sb-Se

Aerosol

3. Source Term Code Package

I-Br*

Cs-Rb*

Te-Sb-Se

Ba

Sr

Ru-Rh-Pd-Tc-Mo

La-Eu-Pr-Nd-Pm-Sm-Y-Nb-Zr(f.p.)

Ce-Np-Pu

In-vessel aerosol

Ex-vessel aerosol

* The transport of these elements is followed as if the masses had the
vapor and chemical properties of CsI or CsOH.