Office of Health, Safety and Security
Operating Experience Level 3

OE-3: 2011-01 **June 2011**

Radcalc V4.1 Software Defect

PURPOSE

This Operating Experience Level 3 (OE-3) report is issued to provide information on software quality assurance problems related to the use of Radcalc V4.1.

BACKGROUND

Radcalc V4.1 is a computer code that has been developed to assist users with various determinations relating to packaging and transportation of radioactive material within the Department of Energy (DOE) complex. One of the functions performed by Radcalc V4.1 is to calculate the partial pressures of hydrogen, oxygen, and helium and the total pressure in the package.

PROBLEM

Based on a report from a Radcalc code user, Energy*Solutions*, Inc. (the code manager) reported errors concerning the calculations of total and partial pressures (hydrogen, oxygen, and helium) in a radioactive waste shipping package. The only Radcalc output affected by the identified problem concerns the hydrogen and helium gas pressure results section. This problem does not affect other Radcalc V4.1 calculations such as Nuclear Regulatory Commission, Department of Transportation and DOE classification results and gas concentration results.

CONCLUSION AND RECOMMENDATIONS

Pressure calculation errors could result in an unanalyzed condition during transportation and potential non-compliance with transportation safety regulations and site administrative safety limits. Users of Radcalc V4.1 should perform and verify their calculations by hand until the errors are corrected in the Radcalc code by the code manager.

The following revised equations should be used to perform the hand calculations and are further described in the Energy*Solutions*, Inc. report PR/CR-078 "Required Revisions to Correct Calculations for Total Pressure in Package and Partial Pressures of Hydrogen, Oxygen, and Helium" available to registered users by accessing the Radcalc web site at https://www.radcalc.energy.gov/.

Partial Pressure of Hydrogen Gas:

$$PP_H = \left(\frac{n_H}{n_{air}}\right) \cdot P_{atm}$$

PP_H = partial pressure of hydrogen gas (Pa)
n_H = moles of hydrogen gas generated once the package is sealed (moles)
n_{air} = moles of air in the package at standard temperature and pressure (moles)
P_{atm} = P_{air} = atmospheric pressure (101325 Pa)

Partial Pressure of Helium Gas:

$$PP_{He} = \left(\frac{n_{He}}{n_{air}}\right) \cdot P_{atm}$$

PP_{He}= partial pressure of helium gas Pascal (Pa)
n_{He} = moles of helium gas generated once the package is sealed (moles)
n_{air} = moles of air in the package at standard temperature and pressure (moles)
P_{atm} = P_{air} = atmospheric pressure (101325 Pa)

Total Pressure in the Package:

$$P_{tot} = \left(\frac{n_{air} + n_H + n_{He}}{n_{air}}\right) \cdot P_{atm} \quad \text{water not present}$$

$$P_{tot} = \left(\frac{n_{air} + n_H + n_O + n_{He}}{n_{air}}\right) \cdot P_{atm} \quad \text{water present}$$

P_{tot} = total pressure in the package (Pa)
n_{air} = moles of air in the package at standard temperature and pressure (moles)
n_H = moles of hydrogen gas generated once the package is sealed (moles)
n_O = moles of oxygen gas generated once the package is sealed (moles)
n_{He} = moles of helium gas generated once the package is sealed (moles)
P_{atm} = P_{air} = atmospheric pressure (101325 Pa)

ADDITIONAL SOURCES OF INFORMATION

The DOE Office of Packaging and Transportation has issued a ***Radcalc Software Safety Alert*** **(DOE/OPT/SA-02)** which has been distributed to registered users and site packaging and transportation personnel. The Alert has been posted on the Radcalc web site at https://www.radcalc.energy.gov/. Questions about Radcalc V4.1 should be directed to the Radcalc Helpdesk at (509) 375-9526 or djlinstrum@energysolutions.com. Questions related to this OE-3 report should be directed to Subir Sen at subir.sen@hq.doe.gov.

Note: There is no action required for past completed waste shipments and packages that have already been opened by the site.

No follow-up report is required to this OE-3 report.

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