



RADCALC SOFTWARE SAFETY ALERT

Issue Number: DOE/OPT/SA-02

Date: May 16, 2011

Problem Report and Correction to Calculate Total and Partial Pressures in a Waste Shipping Package

The Problem:

An error in the transportation software (Radcalc Version 4.1) concerning calculations for total and partial pressures (hydrogen, oxygen, and helium) in a radioactive waste shipping package has been discovered. **The only output affected by the identified problem concerns the “Hydrogen/Helium Gas Results” section which is provided last in the Radcalc 4.1 output.** This problem does not affect other Radcalc 4.1 output such as Classification Results and Gas Concentration Results.

The identified problem concerns how Radcalc 4.1 calculates and provides the output provided under “Pressure When Opened.” The total and partial pressures reported by Radcalc 4.1 in this section have been found to be non-conservative. Any safety or regulatory determinations made using these pressures (e.g., comparison to a package design pressure limit) should be reviewed for potential non compliance. Please refer to the output example as well as additional information for performing hand calculations, provided in **Attachment 1** to this Safety Alert.

NOTE: There are no known issues with using Radcalc 4.1 software to perform transportation classifications. Radcalc 4.1 conservatively calculates and continues to provide **correct** outputs for “Department of Transportation (DOT) Classification Results,” “Department of Energy (DOE) Classification Results,” and “Nuclear Regulatory Commission (NRC) Classification Results.”

Significance of Error:

Error in the pressure calculations for a radioactive waste package could result in the possibility of an unanalyzed condition of transport, and a potential non compliance with transport safety regulations and site administrative safety limits.

Background:

Radcalc is a user-friendly NQA-1 validated software program developed to assist DOE sites' packaging and transportation personnel in packaging and transportation determinations (*e.g. regulatory classification, decay heat, radioactivity, and hydrogen gas generation*) for shipment of radioactive materials and waste. The DOE Office of Packaging and Transportation (EM-45) manages the program through contract with Project Enhancement Corporation and its subcontractor EnergySolutions, Inc. Radcalc 4.1 is safety system software classified as Safety Level B under the

EnergySolutions Software Management Quality Assurance Procedure. Radcalc 4.1 software registration and necessary operating and training documents are available to approved registered users via the web site operated by the Environmental Management Consolidated Business Center in Cincinnati, Ohio.

Proposed Disposition/Corrective Action:

Not all users utilize Radcalc 4.1 methodology to calculate gas generation in the radioactive waste shipping package. The best immediate solution for users that do need to calculate gas generation is to perform the simple pressure calculations independently (**by hand**). The equations to remedy this problem are provided in **Attachment 1** as well as PR/CR-078, "Required Revisions to Correct Calculations for Total Pressure in Package and Partial Pressures of Hydrogen, Oxygen, and Helium," developed by EnergySolutions and distributed to all Radcalc 4.1 approved registered users effective April 27, 2011. The PR/CR document is also available under the "downloads" menu tab located on the website at <https://www.radcalc.energy.gov/dnnradweb/>

What should sites know and do about the proposed correction?

DOE sites **not using** Radcalc 4.1 methodology to determine gas generation in a waste shipping package do not need to take any action.

DOE sites **using** Radcalc 4.1 methodology to determine gas generation in the waste shipping package must take the following actions to assure safety of waste package in preparation, or in transit, or arrived and not opened at the destination site:

- Determine if the calculation(s) in question have been or are being used in your application of Radcalc 4.1.
- If the problem **does not** affect your use of Radcalc 4.1, document or place a notice on the software to this effect that identifies the identified error is not of issue with Radcalc 4.1 usage currently being performed.
- If the problem **does** affect your use of Radcalc 4.1, review current usage in determining pressure in waste packages and perform the following:
 - Via use of hand calculations or other suitable methods, confirm that no error was introduced in determining waste package pressure. If any error is introduced, take appropriate corrective action.
 - For current waste shipping packages under preparation for transportation, use correct methodology described in **Attachment 1** as well as PR/CR-078 available on Radcalc 4.1 website.
- Users must independently check and verify their calculations in accordance with their approved Quality Assurance Programs and Procedures.
- There is no action required for past completed waste shipments and packages that have already been opened by the site.

What will the Office of Packaging and Transportation do about the proposed correction?

The Office of Packaging and Transportation will ensure the proposed change in gas generation methodology is incorporated in the next revision of the Radcalc software.

Need more information?

If you need additional information, please contact Ashok Kapoor, EM-45 at 202-586-8307 or via e-mail at ashok.kapoor@hq.doe.gov or the Radcalc Helpdesk at 509-375-9526 or via e-mail at: djlinstrum@energysolutions.com

ATTACHMENT 1

An example Radcalc 4.1 output for hydrogen/helium gas is provided below. The specific area of concern is shaded. The areas above this shaded area provide no known problems and calculate correctly.

To properly perform hydrogen/helium gas calculations and correctly interpret the results, a detailed knowledge of the physics of hydrogen-gas (H2) and helium (He) generation is required. Only qualified personnel should perform gas pressure calculations. Users must independently check and verify their calculations in accordance with their approved Quality Assurance Programs and Procedures.

****EXAMPLE ONLY****

===== Hydrogen/Helium Gas Results =====

Note - Hydrogen/Helium gas calculations are performed at the end of the user-specified seal time.

Hydrogen Gas:

H2 Concentration:	1	%	
H2 Moles :	17	moles	
H2 Volume :	381000	cm ³	(0 C, 101.325 kPa)
H2 Rate When Sealed:	8.469	cm ³ /hr	(0 C, 101.325 kPa)
H2 Rate When Opened:	8.898	cm ³ /hr	(0 C, 101.325 kPa)

Helium Gas:

He Concentration:	0.0021	%	
He Moles :	0.0003959	moles	
He Volume :	8.873	cm ³	(0 C, 101.325 kPa)
He Rate When Sealed:	0.0001973	cm ³ /hr	(0 C, 101.325 kPa)
He Rate When Opened:	0.0002071	cm ³ /hr	(0 C, 101.325 kPa)

[NOTE: THE INFORMATION SHADED AND IDENTIFIED BELOW IS WHERE THE STATED PROBLEM IN RADCALC 4.1 OCCURS]

Pressure When Opened:

Partial Pressure (H2):	89.57	kPa	
Partial Pressure (He):	0.002086	kPa	
Partial Pressure (O2):	44.78	kPa	(if H2O present in waste)
Total Pressure (H2 + He + Air):	190.9	kPa	
Total Pressure (H2 + He + O2 + Air):	235.7	kPa	(if H2O present in waste)

****EXAMPLE ONLY****

Future use of Radcalc 4.1 is acceptable for all calculations except for hydrogen and helium gas pressure calculations. Please refer to information that follows in Table 1 below when performing these types of calculations. This information has been independently verified.

Table 1. Pressure Calculation Requirements.

Step	Calculation Currently in Radcalc 4.1	Calculation to Resolve Incorrect Radcalc 4.1 Calculation
<p>1.</p>	<p>Radcalc 4.1 shall calculate the volume of air at STP within the package using the equation below:</p> $V_{air} = V_{cv} + \begin{cases} V_{wv} & \text{Waste Void method} \\ V_w - M_w / \rho_w & \text{True Density method} \end{cases}$ <p>where:</p> <p>V_{air} = volume of air (m³) V_{cv} = container void volume (m³) V_{wv} = waste void volume (m³) V_w = waste volume (m³) M_w = waste mass (kg) ρ_w = true (theoretical) density of the waste (kg/m³) STP = standard temperature (0 °C) and atmospheric pressure (101325 Pa)</p>	<p>Radcalc 4.1 performs this calculation correctly.</p>
<p>2.</p>	<p>Radcalc 4.1 shall calculate the moles of air using the equation below:</p> $n_{air} = \frac{V_{air}}{V_m}$ <p>where:</p> <p>n_{air} = quantity of air (moles) V_m = molar volume of an ideal gas at STP (0.022413996 m³/mole)</p>	<p>Radcalc 4.1 performs this calculation correctly.</p>

Table 1. Pressure Calculation Requirements.

Step	Calculation Currently in Radcalc 4.1	Calculation to Resolve Incorrect Radcalc 4.1 Calculation
<p align="center">3.</p>	<p>Radcalc 4.1 shall calculate the partial pressure of hydrogen gas depending on whether water is present using the equations below:</p> $PP_H = \frac{n_H}{(n_H + n_{He} + n_{air})} P_{atm}$ $PP_{HW} = \frac{n_H}{(n_H + n_O + n_{He} + n_{air})} P_{atm}$ <p>where:</p> <p>PP_H = partial pressure of H₂ gas (Pa) PP_{HW} = partial pressure of H₂ gas if water is present (Pa) n_H = H₂ gas accumulated (moles) n_O = total quantity of oxygen generated (moles) if water is present n_{He} = total quantity of helium generated (moles) P_{atm} = atmospheric pressure (101325 Pa)</p>	<p>Replace the equation to the left for calculating the partial pressure of hydrogen gas depending on whether water is present by performing the following hand calculation:</p> $PP_H = \left(\frac{n_H}{n_{air}} \right) \cdot P_{atm}$ <p>where:</p> <p>PP_H = partial pressure of H₂ gas (Pa) n_H = moles of H₂ gas generated once the package is sealed n_{air} = moles of air in the package at standard temperature and pressure P_{atm} = PP_{air} = atmospheric pressure (101325 Pa)</p>
<p align="center">4.</p>	<p>Radcalc 4.1 shall calculate the partial pressure of oxygen gas if water is present using the equation below:</p> $PP_O = \frac{PP_H}{2}$ <p>where:</p> <p>PP_O = partial pressure of O₂ gas (Pa) if water is present</p>	<p>Radcalc 4.1 performs this calculation correctly.</p>

Table 1. Pressure Calculation Requirements.

Step	Calculation Currently in Radcalc 4.1	Calculation to Resolve Incorrect Radcalc 4.1 Calculation
<p>5.</p>	<p>Radcalc 4.1 shall calculate the partial pressure of helium gas using the equation below:</p> $PP_{He} = \frac{n_{He}}{(n_H + n_{He} + n_{air})} P_{atm}$ $PP_{HeW} = \frac{n_{He}}{(n_H + n_O + n_{He} + n_{air})} P_{atm}$ <p>where:</p> <p>PP_{He} = partial pressure of helium gas (Pa) PP_{HeW} = partial pressure of helium gas (Pa) if water is present</p>	<p>Replace the equation to the left for calculating partial pressure of helium gas by performing the following hand calculation:</p> $PP_{He} = \left(\frac{n_{He}}{n_{air}} \right) \cdot P_{atm}$ <p>where:</p> <p>PP_{He} = partial pressure of helium gas (Pa) n_{He} = moles of helium gas generated once the package is sealed n_{air} = moles of air in the package at standard temperature and pressure P_{atm} = PP_{air} = standard atmospheric pressure (101325 Pa)</p>
<p>6.</p>	<p>Radcalc 4.1 currently calculates the total pressure in the package and provides this information as output. However, Radcalc 4.1 performs this incorrectly due to the identification of the above issues.</p> <p>The total pressure in the package is calculated by adding the partial pressures of air, hydrogen, helium and oxygen (if water is present).</p> <p>Users shall perform the calculation provided on the right for obtaining the total pressure in the package.</p>	<p>Perform the following hand calculation to obtain the total pressure in the package:</p> $P_{tot} = \left(\frac{n_{air} + n_H + n_{He}}{n_{air}} \right) \cdot P_{atm} \quad \text{water not present}$ $P_{tot} = \left(\frac{n_{air} + n_H + n_O + n_{He}}{n_{air}} \right) \cdot P_{atm} \quad \text{water present}$ <p>where:</p> <p>P_{tot} = total pressure in the package (Pa) n_{air} = moles of air in the package at standard temperature and pressure n_H = moles of hydrogen gas generated once the package is sealed n_O = moles of oxygen gas generated once the package is sealed n_{He} = moles of helium gas generated once the package is sealed P_{atm} = PP_{air} = standard atmospheric pressure (101325 Pa)</p>