LANL '08 TA-21 SWMU 21-018(a)-99 (MDA V)
ENTER

Roberts, Kathryn, NMENV

From: Charles J. English [cenglish@lanl.gov]
Sent: Wednesday, May 21, 2008 3:20 PM
To: dgregory@doeal.gov
Cc: Roberts, Kathryn, NMENV; bcriswell@lanl.gov; rrager@lanl.gov
Subject: Re: Calculation for tritium activity in pore water

Attachments: h-3 conversion 5-21-08.doc

h-3 conversion 5-21-08.doc (56...

David,

Attached is the information Katie asked for concerning the tritium calculations. This includes a complete derivation of the equation presented in the NOD response, along with supporting information concerning one of the key assumptions.

I have copied Katie with this response. Please let me know if you have any questions.

Joe

> From: Roberts, Kathryn, NMENV [mailto:Kathryn.Roberts@state.nm.us] Sent: Friday, May 16, 2008 8:00 AM
> To: Gregory; Criswell; cenglish@lanl.gov
> Cc: Cobrain, Dave, NMENV; Shen, Hai, NMENV
> Subject: Calculation for tritium activity in pore water
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> Joe,
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>
> Could you please send your complete derivation of the equation
> included in
> specific comment # 4 of the MDA V NOD Response? Understanding the assumptions that you used would help us respond to the comment more appropriately.
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> If possible, please have this information to us by Monday afternoon.
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> If you have any questions feel free to contact me.
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> Thanks,
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> Katie
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>
>
> Kathryn Roberts
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Conversion of Tritium Activity in Pore Water to Activity in Tuff

Given:

Specific activity of tritium in pore water as determined by pore gas sampling (i.e., activity of tritium per unit volume of pore water).

Find:

Specific activity of tritium in bulk tuff sample (i.e., activity of tritium per unit weight of tuff).

Assumptions:

1. Total porosity of tuff is 0.45 (range of 0.40 to 0.67 reported in Table 4.9-1 of MDA V Investigation Report, Rev. 1).

2. Volumetric moisture content is 0.10 (based on median value of gravimetric moisture content reported in Table 4.9-1 of MDA V Investigation Report, Rev. 1 – see Attachment 1).

3. Dry density of tuff is 1.46 g/cm^3 (range of 0.87 to 1.59 reported in Table 4.9-1 of MDA V Investigation Report, Rev. 1).

4. Inventory of tritium is present only in pore liquid; vapor phase inventory in pore gas is negligible (see Attachment 1).

Solution:

Specific activity of tritium in tuff is equal to total activity of tritium in given amount of tuff divided by the dry weight of the tuff:

$$SA = \frac{A}{W_{tuff}} \qquad \text{Eq. 1}$$

Where SA = specific activity of tritium in tuff on dry weight basis (pCi tritium per g dry tuff),

A = total activity of tritium in given amount of tuff (pCi tritium), and

W_{tuff} = dry weight of tuff (g tuff).

The total activity of tritium in a given amount of tuff is equal to the volume of pore water present in the tuff multiplied by the specific activity of tritium in the water.

$$A = V_{water}\, T_{water} \qquad \text{Eq. 2}$$

Where V_{water} is the volume of water (L water) and

T_{water} is the specific activity of tritium in water (pCi tritium per L water).

The volume of water is equal to the volume of tuff multiplied by the volumetric moisture content.

$$V_{water} = V_{tuff}\,\theta_{water} \qquad \text{Eq. 3}$$

Where V_{tuff} is the volume of tuff (L tuff) and

θ_{water} is the volumetric moisture content of the tuff (L water per L tuff).

Substituting Eq. 3 in Eq. 2 gives:

$$A = V_{tuff}\,\theta_{water}\,T_{water} \qquad \text{Eq. 4}$$

The dry weight of tuff is equal to the volume of tuff multiplied by the dry density of tuff:

$$W_{tuff} = V_{tuff}\,\rho_{tuff} \qquad \text{Eq. 5}$$

Where ρ_{tuff} = dry density of tuff (g tuff per cm^3 tuff).

Substituting Eq. 4 and Eq. 5 in Eq. 1 gives:

$$SA = \frac{V_{tuff}\,\theta_{water}\,T_{water}}{V_{tuff}\,\rho_{tuff}} \qquad \text{Eq. 6}$$

Simplifying Eq. 6 gives

$$SA = \frac{\theta_{water}\,T_{water}}{\rho_{tuff}} \qquad \text{Eq. 7}$$

Eq. 7 is then used to calculate the specific activity of tritium:

$$\frac{\left(0.1\,{}^{L_{water}}/_{L_{tuff}}\right)\left(132{,}100\,{}^{pCi}/_{L_{water}}\right)}{\left(1.46\,{}^{g_{tuff}}/_{cm^3_{tuff}}\right)\left(1000\,{}^{cm^3_{tuff}}/_{L_{tuff}}\right)} = 9.05\,{}^{pCi}/_{g_{tuff}}$$

Attachment 1 – Partitioning of Tritium Between Liquid and Vapor Phases in the Subsurface

The tritium detected in pore gas samples is present as tritiated water (HTO or T_2O), which is essentially identical to normal water (H_2O) in terms of chemical and physical properties (other than molecular weight). This tritiated water will be present within pore spaces in soil and tuff as liquid water and water vapor. The amount of water present within the pore spaces depends on the moisture content of the soil or tuff. Geotechnical characterization samples collected during the MDA V investigation show the tuff beneath MDA V to have low moisture contents and high porosities (Investigation Report, Table 4.9-1). Thus, pore spaces will mainly be filled with air.

The water vapor in the air within pore spaces in subsurface media should be in equilibrium with liquid water, resulting in saturated conditions (i.e., 100% relative humidity). The actual amount of water vapor present per volume of pore space is the absolute humidity, which is a function of temperature and pressure. Under conditions typical of the subsurface at MDA V (temperature 15°C, absolute pressure 800 mbar, 100% relative humidity), the absolute humidity is 12.85 g/m^3 (http://www.vaisala.com/humiditycalculator/). The absolute humidity and the geotechnical properties of the tuff can be used to determine the relative partitioning of tritium between the vapor and liquid phases. Geotechnical properties of tuff were determined as part of the MDA V investigation. Median values reported in Table 4.9-1 of the MDA V Investigation Report are:

- Density – 1.24 g/cm^3
- Gravimetric moisture content – 7.9%
- Total porosity – 53.2%

The mass of liquid-phase water per unit volume of tuff can be calculated as the product of the dry tuff density and the gravimetric moisture content:

$$W_L = (1.24\, {}^{g_{tuff}}\!/_{cm^3_{tuff}})\,(0.079\, {}^{g_{liquid\ water}}\!/_{g_{tuff}}) = 0.098\, {}^{g_{liquid\ water}}\!/_{cm^3_{tuff}}$$

This result can be divided by the density of water to get the volumetric moisture content:

$$V_W = \frac{0.098\, {}^{g_{liquid\ water}}\!/_{cm^3_{tuff}}}{1.0\, {}^{g_{liquid\ water}}\!/_{cm^3_{liquid\ water}}} = 0.098\, {}^{cm^3_{liquid\ water}}\!/_{cm^3_{tuff}}$$

The mass of vapor-phase water per unit volume of tuff can be calculated as the difference between the total porosity and volumetric moisture content (i.e., the air-filled porosity) and the absolute humidity:

$$W_V = \left(0.532\,{cm^3_{air+water}}/{cm^3_{tuff}} - 0.098\,{cm^3_{water}}/{cm^3_{tuff}}\right)\left(12.85\,{g_{water}}/{m^3_{air}}\right)\left(1x10^{-6}\,{m^3_{air}}/{cm^3_{air}}\right) =$$

$$0.0000056\,{g_{water\ vapor}}/{cm^3_{tuff}}$$

The mass percentage of water present in the liquid phase is:

$$P_W = \frac{0.098\,{g_{liquid\ water}}/{cm^3_{tuff}}}{0.098\,{g_{liquid\ water}}/{cm^3_{tuff}} + 0.0000056\,{g_{water\ vapor}}/{cm^3_{tuff}}} 100\% = 99.99\%$$

This partitioning shows that virtually all of the mass of water (and tritium) is associated with the liquid phase.