576464

Sandia National Laboratories

Operated for the United States Department of Energy
by National Technology and Engineering Solutions
of Sandia, LLC.

Carlsbad, NM 88220

date: December 20, 2021

to: Records Center

from: Seth King (08881) *Signature on File*

subject: Methodology for Calculating Initial Waste Area Pressure in the Salado Flow Calculation

Microbial gas-generation rates from the consumption of cellulosic, plastic, and rubber (CPR) materials in the WIPP were determined from 10 years of experimental data gathered at Brookhaven National Laboratory (BNL) (Francis et al. 1997). The rate of microbial gas generation was shown to decrease significantly over the 10-year experimental period. The CPR biodegradation model in the Salado Flow calculation of the performance assessment (PA) is based on the long-term rates found in the BNL experiments.

Nemer et. al. (2005) calculated the additional moles of gas that would be generated during the initial high gas-generation rate time period. The additional moles of gas are then converted to a pressure increase based on the ideal gas equation of state using the repository volume and porosity. At repository closure, the non-waste excavated areas in the repository are initialized at atmospheric pressure. To account for the additional pressure from the early high gas-generation rate, in the waste areas the pressure is initialized to atmospheric pressure plus the additional pressure increase calculated by Nemer et. al. (2005). The calculation performed by Nemer et. al. (2005) solves for the initial gas pressure as a function of the CPR inventory and waste storage volume.

With every new Performance Assessment Inventory Report (PAIR), the CPR inventory is changed. This CPR inventory has been small, and the initial pressure calculation has not been updated. With the Department of Energy (DOE) evaluating options for additional waste storage volumes, the initial pressure was updated by King (2020) to account for the additional repository volume, however the calculation was not updated to account for changes to the CPR inventory since the Nemer et. al. (2005) calculation. With DOE considering different options for repository layout, it has been determined that the best path forward for the initial pressure calculation is to define an early gas-generation rate and recalculate the initial pressure with the repository volume and CPR used for the PA following the methodology described by Nemer et al. (2005).

Nemer et al. (2005) found that the early time gas-generation produced 181 μmol/g cellulose over 481 days. A correction factor of 1.56 was applied to the rate to account for the CO_2 dissolved in the brine (Wang and Brush, 1996). There are 6 moles of organic carbon (and therefore CO_2) per mole of cellulose ($C_6H_{10}O_5$), the molar mass of cellulose is 162 g/mole, and 1 mole of gas produced for every 2 moles of organic carbon. These values were used in Equation 15 of Nemer et al. (2005) along with the mass of CPR in the inventory to calculate the number of moles of gas produced (M_{gas}). For the updated calculation, Equation 15 of Nemer et al. (2005) is modified such that (M_{gas}) is left as a function of CPR mass (M_{cpr}):

$$M_{gas} = 181 \times 10^{-6} \frac{mol\ CO_{2(g)}}{g\ cell} \times 1.56 \frac{mol\ CO_2}{mol\ CO_{2(g)}} \times \frac{1000\ g\ cell}{1\ kg\ cell} \times \frac{1\ mol\ gas}{2\ mol\ CO_2} \times M_{cpr}$$

$$= 0.14118 \frac{mol\ gas}{kg\ cell} M_{cpr} \quad (1)$$

Information Only

Changes were made to the calculation from Nemer et al. (2005) because inventory is typically provided in mass (kg) of CPR (rather than moles of C)—as a result, the values of 6 moles C/mole cellulose and 162 g/mole are not included. Given equation (1), it is recommended the waste storage area initial pressure (CAVITY1:PRESSURE and CAVITY2:PRESSURE) in the PA parameter database be reset to atmospheric pressure (101,325 Pa) and a new PA parameter be defined (WAS_AREA:EGRATMIC) as a constant value of 1.4118×10^{-1} moles (of gas) per kilogram (of cellulose). The description of the new parameter WAS_AREA:EGRATMIC should read "Moles of gas generated per kilogram of cellulose from early-time rapid CPR bio-degradation."

With these values in the parameter database, in the first ALGEBRACDB step of the BRAGFLO calculation, the total moles of gas can now be calculated as:

$$MC_EGAS = (WAS_AREA{:}\,EGRATMIC) \times (WTCELTOT + WTRPLTOT) \quad (2)$$

Where *MC_EGAS* is the moles of early gas, *WTCELTOT* is the mass of cellulose and *WTRPLTOT* is the mass of Rubber and Plastic. Note that this calculation continues to assume the early time CPR gas generation involves degradation of Plastic and Rubber independently of the sample parameter (WAS_AREA:PROBDEG) which impacts Plastic and Rubber biodegradation for long-term gas generation.

With the moles of gas generated from early time CPR biodegradation, an increase in pressure can be calculated with the idea equation of state:

$$\Delta P\ (Pa) = \frac{M_{gas} RT}{V} \quad (3)$$

Where M_{gas} is the moles of gas generated, R is the ideal-gas constant (8.31451 kg m^2/(mol sec K), T is the repository temperature (T=293 K), and V is the pore space volume of the repository:

$$V = (REFCON{:}\,VREPOS) * (WAS_AREA{:}\,POROSITY) \quad (4)$$

Using this calculation, the pressure at repository closure can be updated to atmospheric plus ΔP from equation (3).

In conclusion, a new PA parameter and two updated parameters are proposed:

Table 1 Proposed Parameter Values

Material	Property	Distribution	Value	Units
WAS_AREA	EGRATMIC	Constant	0.14118	Moles per kg
CAVITY1	PRESSURE	Constant	101,325	Pa
CAVITY2	PRESSURE	Constant	101,325	Pa

It is then recommended the pressure at repository closure can be calculated in the first ALGEBRACDB step of the Salado Flow calculation using equations (2) through (4).

Information Only

References

Francis, A. J., J. B. Gillow and M. R. Giles. 1997. Microbial Gas Generation Under Expected Waste Isolation Pilot Plant Repository Conditions. Sandia National Laboratories, Albuquerque, NM. SAND96-2582. ERMS#244883.

King, S. 2020. Initial Waste Area Pressure for the Additional Panels Performance Assessment. Sandia National Laboratories. Carlsbad, NM. ERMS 574357.

Nemer, M., J. Stein, W. Zelinski. 2005. Analysis Report for BRAGFLO Preliminary Modeling Results With New Gas Generation Rates Based Upon Recent Experimental Results. Sandia National Laboratories. Carlsbad, NM. ERMS 539437.

Wang, Y., and L. Brush (1996). Estimates of Gas-Generation Parameters for the Long-Term WIPP Performance Assessment. Memorandum to Martin S. Tierney, January 26. Sandia National Laboratory, Albuquerque, NM. ERMS 231943.

WIPP:4.2.1:PA:QA-L:576427

Information Only