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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Report for BRAGFLO Modeling Results with the removal of Methanogenesis from the Microbial-Gas-Generation Model

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1 EXECUTIVE SUMMARY

The U.S. Environmental Protection Agency (EPA) has directed, during its review of the first Compliance Recertification Application (CRA) by the U.S. Department of Energy (DOE), that the Waste Isolation Pilot Plant (WIPP) Performance Assessment (PA) will assume that all microbial gas generation occurs by denitrification and sulfate reduction. Methanogenesis is to be removed from the microbial gas generation model, because the EPA believes that excess SO_4 may be available at all times in the repository from the disturbed rock zone. Methanogenesis only occurs when availability of NO_3 and SO_4 limits denitrification and sulfate reduction.

This analysis was conducted to perform an assessment of the potential effects on pressure, brine saturation and brine outflow of removing methanogenesis from WIPP PA modeling. The stoichiometry of gas generation without methanogenesis is very similar to the CRA in which methanogenesis is the dominant gas generation reaction. Consequently, differences in repository behavior (pressure, brine saturation, and brine outflow) from the CRA are not significant.

2 INTRODUCTION AND OBJECTIVES

In 1996, the U.S. Department of Energy (DOE) completed a performance assessment (PA) for the certification of the Waste Isolation Pilot Plant (WIPP). Performance Assessment was part of the Compliance Certification Application (CCA) (DOE, 1996) submitted to the Environmental Protection Agency (EPA) to demonstrate compliance with the long-term radioactive disposal standards of 40 CFR 191 (subparts B and C) (EPA, 1993) and the associated certification criteria of 40 CFR 194 (EPA, 1996). Based on the CCA and subsequent information and analyses, the EPA certified WIPP's compliance in May of 1998. As required by the WIPP Land Withdrawal Act (Public Law 102-579 [as amended by Public Law 104-201]) (U.S. Congress 1992, 1996), DOE is required to submit documentation of continued compliance to EPA for the recertification of the WIPP every five years following the first receipt of waste.

The DOE submitted its first Compliance Recertification Application (CRA) in March, 2004 (DOE, 2004). During their review for completeness, the EPA stipulated in comment G-14 of the third completeness letter that if "new and convincing" evidence for methanogenesis cannot be cited, then the DOE must assume that degradation of organic materials will only occur by denitrification and sulfate reduction (EPA, 2004). The purpose of this analysis is to assess the potential effects of the removal of methanogenesis on BRAGFLO results (e.g. pressure, brine saturation, and brine outflow). Effects on the chemical environment are not considered.

3 APPROACH

This analysis was conducted in accordance with Analysis Plan AP-112, which provides direction for "activities used to perform and document CRA submittal analyses and to generate responses to EPA CRA information requests" (Kirkes and Wagner, 2004). Herein we present a preliminary assessment of the effects of removing methanogenesis from the gas-generation calculations on pressure, brine saturation, and brine outflow from BRAGFLO calculations, which are the main output variables that affect subsequent PA analyses. Brine saturation and pressure are used in DBR and SPALLINGS PA analyses, and brine outflow is used in flow and transport analyses.

Two scenarios, S1 and S2, are used in this analysis, which fully encompass the range of results and conditions of all six scenarios from the CRA (Stein and Zelinski, 2003). Scenario S1 is the undisturbed base case, which is a baseline for most PA analyses. Scenario S2 involves a drilling penetration at 350 years through the waste panel into a pressurize brine pocket in the Castile formation. Scenario S2 produced the highest brine outflows in CRA. Each scenario consists of 100 vectors of sampled parameters.

4 METHODOLOGY

4.1 Gas Generation Chemistry

The conceptual model for microbial-gas generation in the CCA/CRA considered three reaction pathways (Wang and Brush, 1996a):

$$C_6H_{10}O_5 + 4.8\ H^+ + 4.8\ NO_3^- \rightarrow 7.4\ H_2O + 6\ CO_2 + 2.4\ N_2 \quad \text{[denitrification]}, \quad (1)$$

$$C_6H_{10}O_5 + 6\ H^+ + 3\ SO_4^{2-} \rightarrow 5\ H_2O + 6\ CO_2 + 3\ H_2S \quad \text{[sulfate reduction]}, \quad (2)$$

Assuming that reactions (1)-(3) proceed sequentially, y_{max} is determined by summing the amount of gas generated by all three reaction pathways

$$y_{\max} = \frac{\frac{2.4M_{NO3}}{4.8} + \frac{3M_{SO4}}{3} + \frac{1}{2}\left(M'_{cel} - \frac{6M_{NO3}}{4.8} - \frac{6M_{SO4}}{3}\right)}{M'_{cel}}, \quad (8)$$

where

M'_{cel} is the quantity (moles) of organic C that potentially will degrade in 10,000 years,

M_{NO3} is the quantity (in moles) of NO_3 initially in the repository,

M_{SO4} is the quantity (in moles) of SO_4 that is available to biodegradation.

Here M'_{cel} is determined from the sampled rates of microbial degradation (Wang and Brush, 1996a)

$$M'_{cel} = \min\left\{\frac{6000M_{cel}}{162}, 10000R'_C \times M_{cel}\right\}, \quad (9)$$

with

$$R'_C = \max\{R_{m,i}, R_{m,h}\}, \quad (10)$$

where

M_{cel} is the quantity (kg) of cellulose initially in the repository,

$R_{m,i}$ is the sampled inundated rate for biodegradation (mol C/year/kg cellulose),

$R_{m,h}$ is the sampled humid rate for biodegradation (mol C/year/kg cellulose).

The minimum value for y is obtained by subtracting the amount of gas consumed by iron-corrosion G,

$$y_{\min} = y_{\max} - \frac{G}{M'_{cel}}. \quad (11)$$

Although iron-corrosion could consume CO_2 to form $FeCO_3$, iron sulfidation shown in equation (5) produces one mol of gas per mol gas consumed. However in the CCA/CRA the H_2S gas was still subtracted from y_{max} to determine y_{min}

$$G = \min\left\{\frac{3M_{SO4}}{3}, M'_{Fe}\right\}, \quad (12)$$

where

M'_{Fe} is the quantity of metal that will potentially degrade in 10,000 years (in moles),

M_{SO4} is the quantity (in moles) of SO_4 that is available to biodegradation.

The amount of iron M'_{Fe} is determined from a method similar to equation (10), Wang and Brush 1996a. Because sulfate reduction accounted for only 2.4% of microbial gas generation in the CRA,

$$C_6H_{10}O_5 + H_2O \rightarrow 3\ CH_4 + 3\ CO_2 \qquad \text{[methanogenesis].} \quad (3)$$

Reactions (1)-(3) are assumed to proceed sequentially, which is the order of decreasing energy yield for the three reactions. Thus methanogenesis occurs after the exhaustion of available nitrate and sulfate.

Some products of reactions (1)-(3) react with magnesium oxide and iron. MgO is added to the repository as backfill to remove CO_2 and to buffer pH. The consumption of CO_2 by MgO is described by the overall reaction (Wang and Brush, 1996b):

$$MgO + CO_{2(aq)} \rightarrow MgCO_3. \quad (4)$$

Iron sulfidation consumes H_2S and produces H_2

$$Fe + H_2S \rightarrow FeS + H_2. \quad (5)$$

The microbial-gas-generation model in BRAGFLO is limited to a single reaction, which is meant to describe the overall decomposition of cellulosics and reactions (4)-(5) in an average stoichiometric model. The overall reaction in this model is represented by

$$C + \text{unknown} \rightarrow y\,H_{2(g)} + \text{unknown}, \quad (6)$$

where y is the amount of gas produced per mol of organic carbon. This model assumes that H_2O is neither produced nor consumed. In BRAGFLO all gas is treated as hydrogen for use in the Redlich-Kwong-Soave equation of state.

Because of uncertainty in the conceptual model, the value of y in each BRAGFLO vector is sampled on a uniform distribution over the range $[y_{min}, y_{max}]$

$$y = y_{min} + \beta \times (y_{max} - y_{min}), \quad (7)$$

where β is a sampled input parameter ($0 \le \beta \le 1$). The value y_{max} is determined by assuming that no microbially-generated gas reacts with steel or steel-corrosion products, y_{min} assumes complete reaction of microbially-generated gas with steel or steel-corrosion products. In section 4.2 we present a derivation of the stoichiometric factor y used in the CRA. A derivation for use in the absence of methanogenesis is presented in section 4.3.

4.2 The Stoichiometric Factor in the CRA (with methanogenesis)

In the CRA (and in this study) the amount of NO_3 initially in the waste limited detrification to about 2.5% of microbial-gas generation. The amount of SO_4 initially in the waste limited gas generation by sulfate reduction to about 1.2%. Methanogensis accounted for about 96.3% of microbial-gas generation.

$G/M'_{cel} << y_{max}$ and thus the error in subtracting the amount of H_2S produced was small and had little impact on repository behavior as will be shown in §5.

4.3 Proposed Stoichiometric Factor in the Absence of Methanogenesis

In the absence of methanogenesis, the value y_{max} was determined by assuming that reaction (1) occurs followed by reaction (2) until all the cellulose is exhausted,

$$y_{max} = \frac{\left[\frac{2.4}{4.8} M_{NO3} + \frac{1}{2}\left(M'_{cel} - \frac{6}{4.8} M_{NO3}\right)\right]}{M'_{cel}}. \qquad (13)$$

Notice that the value of y_{max} in equation (13) is unchanged from the value in equation (8). This occurs because reaction pathways (2) and (3) are equivalent in terms of the amount of gas produced per mol of organic carbon, in the absence of CO_2. Each pathway produces 1 mol gas per 1 mol cellulose.

In the absence of methanogenesis, the value of y_{min} was set equal to y_{max} because reaction (5) produces one mol of gas per mol of gas consumed,

$$y = y_{max}. \qquad (14)$$

Thus y and β are no longer sampled input parameters.

4.4 Implementation in BRAGFLO

The new values of y_{max} and y_{min} given by equations (13)-(14) were implemented in BRAGFLO by altering the ALGEBRA1 input file, which is a preprocessing step before the BRAGFLO simulation is run. This was accomplished with the following changes:

CRA

```
NUM2 = MAKEPROP(3*MOL_SO4/3)
NUM3 = MAX_CELL - 6*MOL_NO3/4.8 - 6*MOL_SO4/3
YMAX = (NUM1+NUM2+0.5*NUM3)/MAX_CELL

C1   = NUM2
C2   = MAX_FE
G    = MIN(C1,C2)
YMIN = YMAX - G/MAX_CELL
```

No methanogenesis

```
NUM3 = MAX_CELL - 6*MOL_NO3/4.8
```

YMAX = (NUM1+0.5*NUM3)/MAX_CELL

G = 0.0
YMIN = YMAX - G/MAX_CELL

4.5 Comparison of BRAGFLO Assumptions With and Without Methanogenesis

The sampled input parameter PROBDEG determines the type of organic material that decomposes to produce gas in each vector. In both the CRA and this analysis, 50% of vectors have no microbial gas generation. In 25% of vectors only cellulosics biodegrade. Cellulosics, plastic and rubber (CPR) biodegrade in the remaining 25% of vectors.

Because the lower bound on the sampled rate of cellulosics biodegradation is large enough to decompose all of the material in 10,000 years, the value of M'_{cel} in equation (9) has only two possible values of interest. These two values correspond to the case where only cellulose biodegrades (PROBDEG = 1), and the case where all CPR biodegrades (PROBDEG=2). Table 1 summarizes the values of y_{min} and y_{max} for the two cases, in the CRA and in the no-methanogenesis implementation.

Table 1. Comparison of Stoichiometric Factors

	Biodegradable Organics	y_{min}	y_{max}
No Methanogenesis	Cellulosics only	0.491	0.491
CRA	Cellulosics only	0.473	0.491
No Methanogenesis	CPR	0.497	0.497
CRA	CPR	0.491	0.497

5 BRAGFLO RESULTS

The changes to the stoichiometric factor, shown in Table 1, resulted in small differences compared to the CRA in pressure, brine saturation, and brine outflow for most vectors. Overall repository performance was not significantly affected. Two methods are used below to present the differences in BRAGFLO simulation results between these no-methanogenesis calculations and the CRA. Scatter plots show simulation results in the case of no methanogenesis versus results from the CRA. Points are plotted for all vectors at times listed in Table 2, which are a representative set of times that spans the entire 10,000-year modeling period. Differences between no-methanogenesis and CRA results are seen by the distance that points lie away from the diagonal line. Plots of max, min and average values of simulation results versus time are also shown for CRA and no-methanogenesis results.

Table 2. Times of points plotted in scatter plots.

Period (years)	Points plotted every (years)
0-500 years	10
500-1000 years	20
1000-10000	100

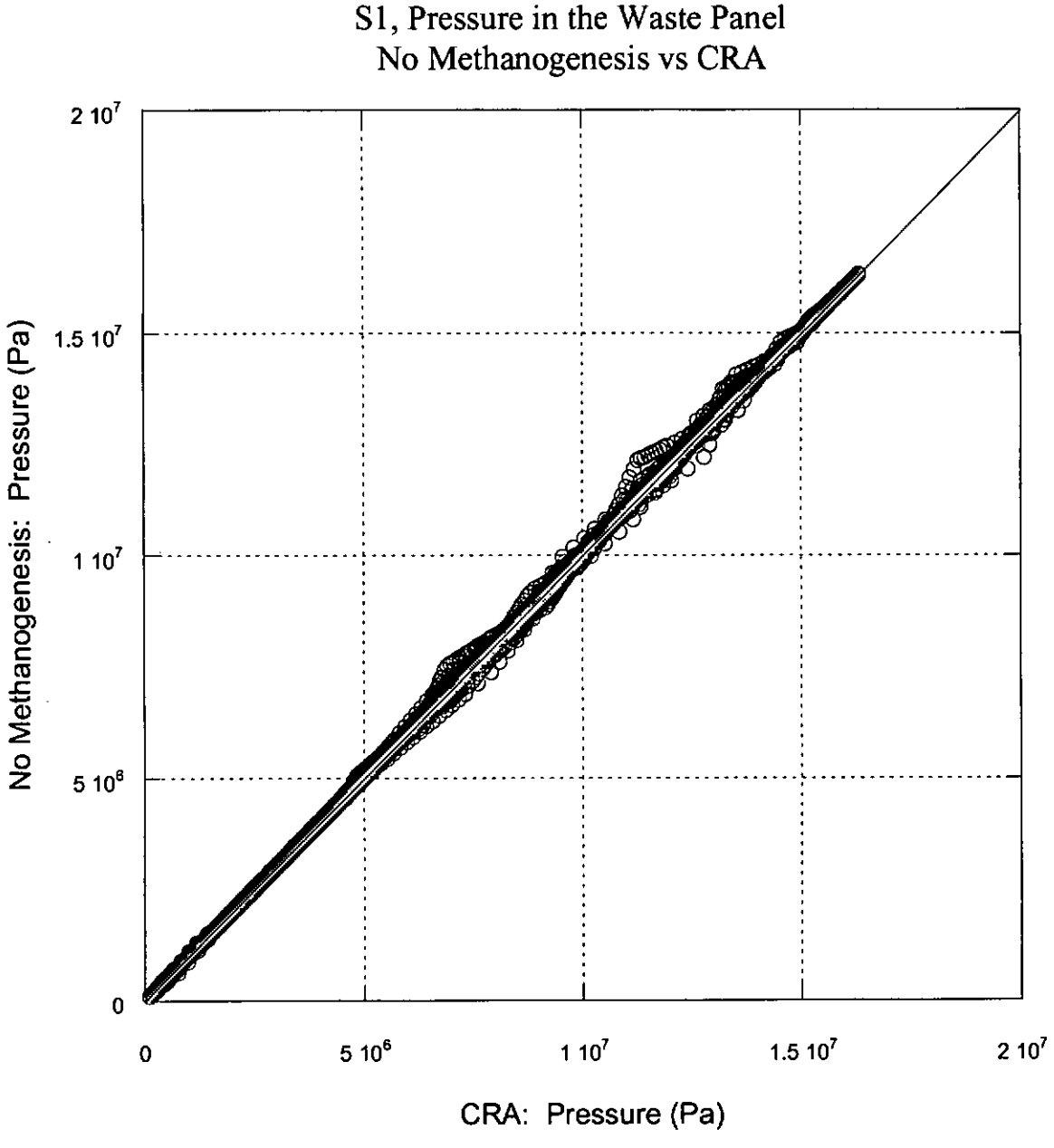

Figure 1. Scatter plot of pressure in the waste panel for scenario S1. Points are pressures from each vector, without methanogenesis versus results obtained from CRA calculations. The times plotted are listed in Table 2.

5.1 Pressure

Figures 1 and 2 are scatter plots of pressure in the waste panel (WAS_PRES) for the no-methanogenesis calculations versus the CRA. The higher stoichiometric factor in some vectors (Table 1) results in more microbial gas generation and higher pressure for some vectors in the no-methanogenesis models. This results in some points above the diagonal line in Figure 1 (S1). Figure

2 (S2) also shows minor dispersion on both side of the line. The differences occur at moderate pressures.

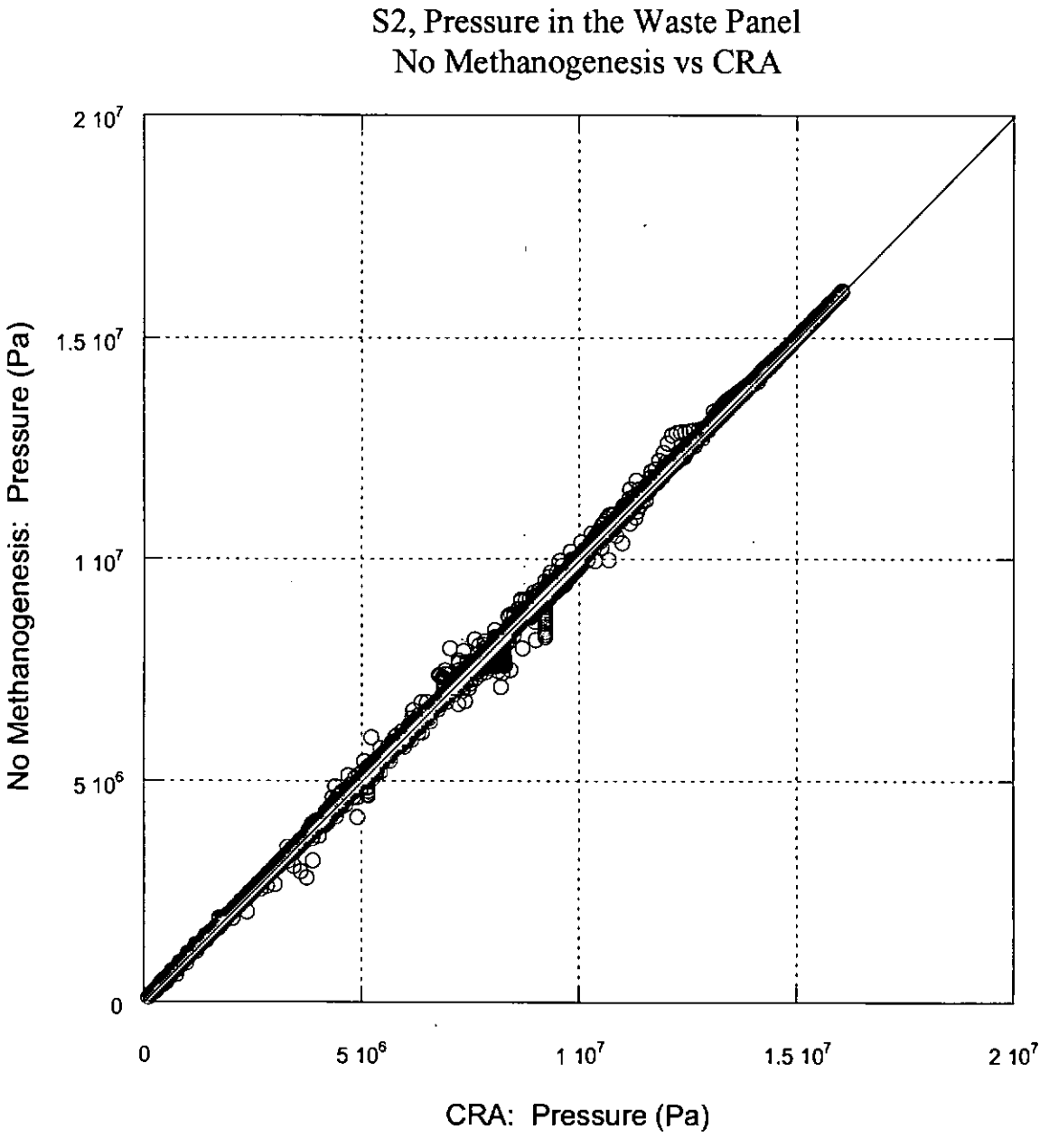

Figure 2. Scatter Plot of pressure in the waste panel for Scenario S2. Points have the same meaning as in Figure 1.

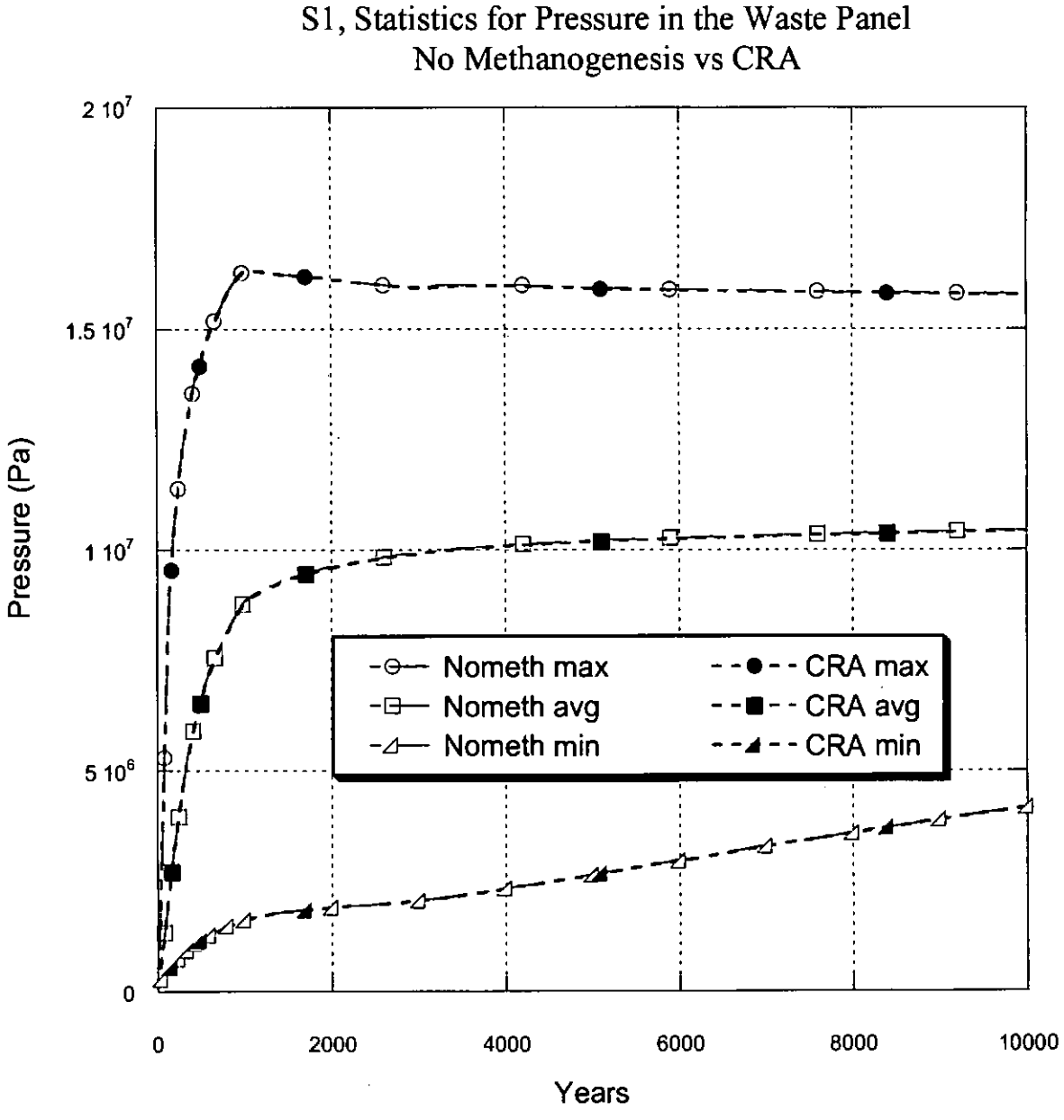

Figure 3. Pressure in the waste panel versus time for scenario S1. Red points and lines represent results without methanogenesis. Black points (lines) represent results from the CRA. The maximum pressure curve is the maximum over all vectors at each time plotted, same for the average and the minimum. The times plotted are listed in Table 2.

Figures 3 and 4 present plots of maximum, minimum, and average pressure for the no-methanogenesis and the CRA versus time. The removal of methanogenesis from the model has no visually discernable effect on the distribution of pressure values throughout 10,000 years in either scenario.

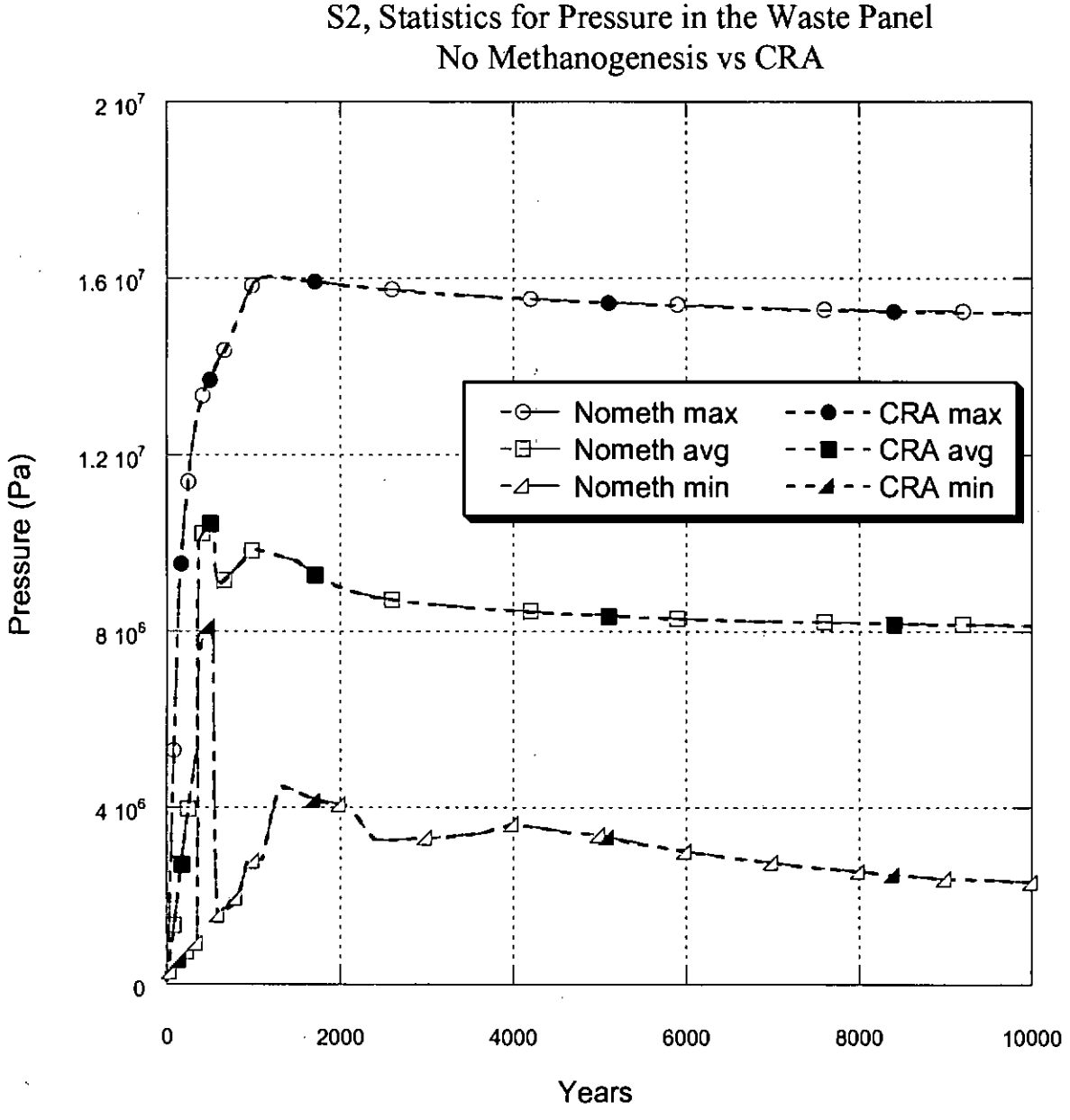

Figure 4. Pressure in the waste panel versus time for scenario S2. Points and colors have the same meanings as in Figure 3.

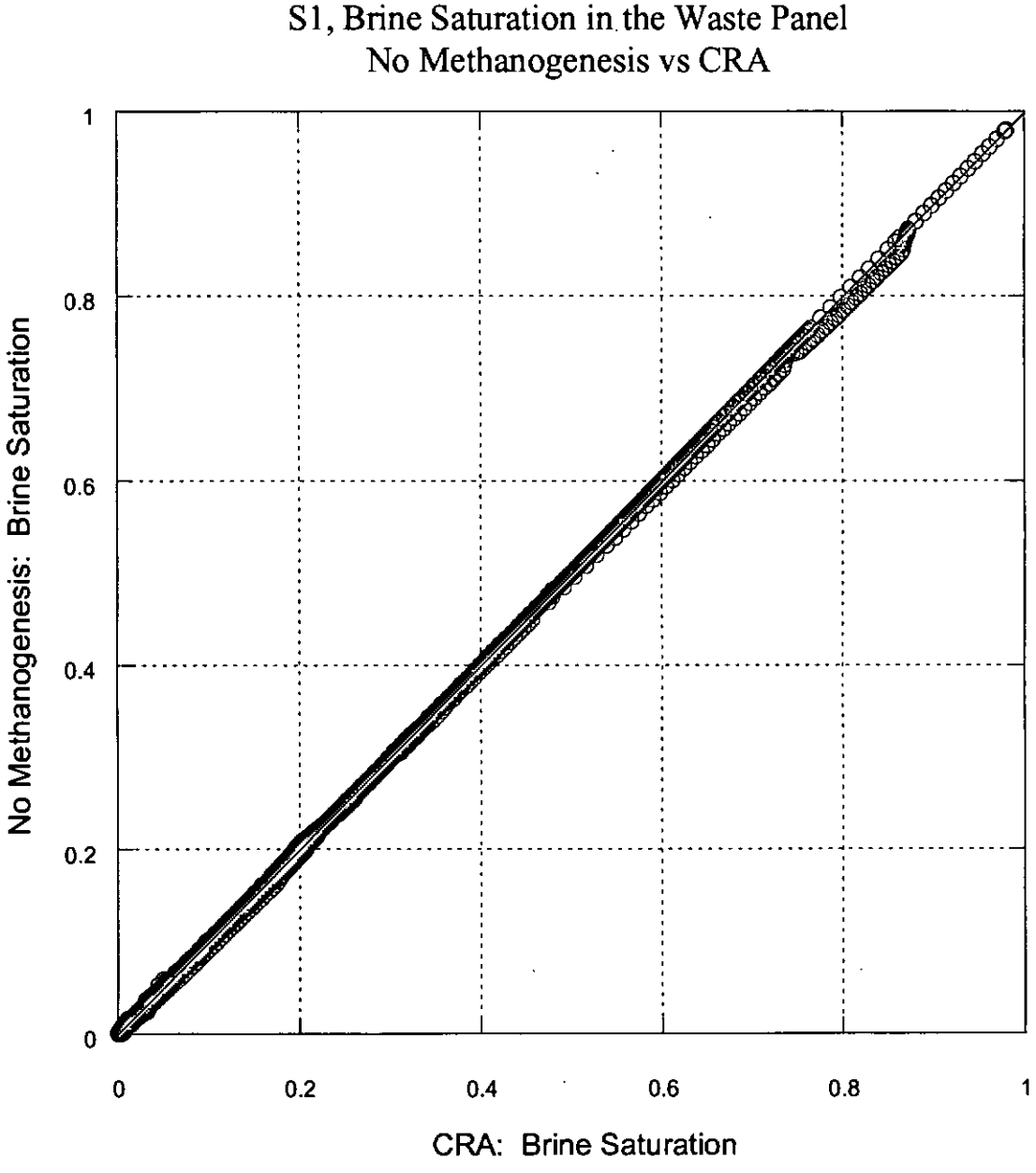

Figure 5. Scatter plot of brine saturation in the waste panel for scenario S1. Points are brine saturations from each vector, without methanogenesis versus that obtained from CRA calculations. The times plotted are listed in Table 2.

5.2 Brine Saturation

Figures 5 and 6 present scatter plots of brine saturation in the waste panel (WAS_SATB) from no-methanogenesis calculations versus the CRA. The vast majority of points in Figure 5 (S1) fall on the diagonal line. The points slightly below the diagonal line represent vectors that had slightly lower stoichiometric factors in the CRA (Table 1) and consequently, slightly higher pressure and lower brine saturation.

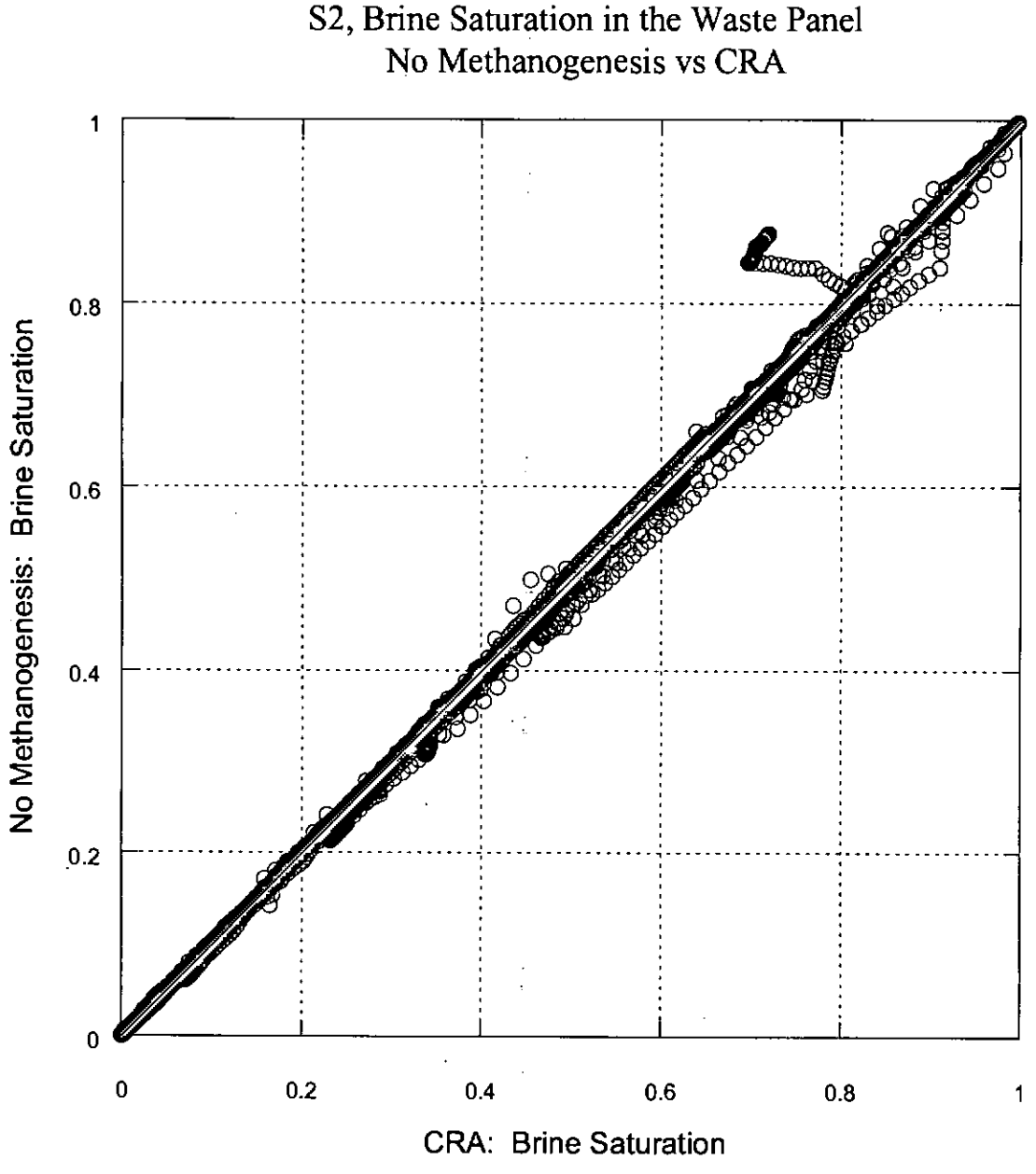

Figure 6. Scatter plot of brine saturation in the waste panel for scenario S2. Points have the same meaning as in Figure 5.

The points below the diagonal line in Figure 6 also represent vectors with lower stoichiometric factors and slightly higher pressure in the CRA.

The anomalous string of points extending above the diagonal line in Figure 6 represents Vector 98 beginning at about 5,000 years (Figure 7). The effect of vector 98 on pressure and brine outflow was negligible (Figures 1 and 10), but brine saturation showed an observable departure of values from the CRA beginning at about 5000 years (Figure 7). Occasionally calculations fail to converge in BRAGFLO models, and it is necessary and normal to adjust convergence parameters. There are three primary convergence adjustments, and vector 98 required two of these adjustments in

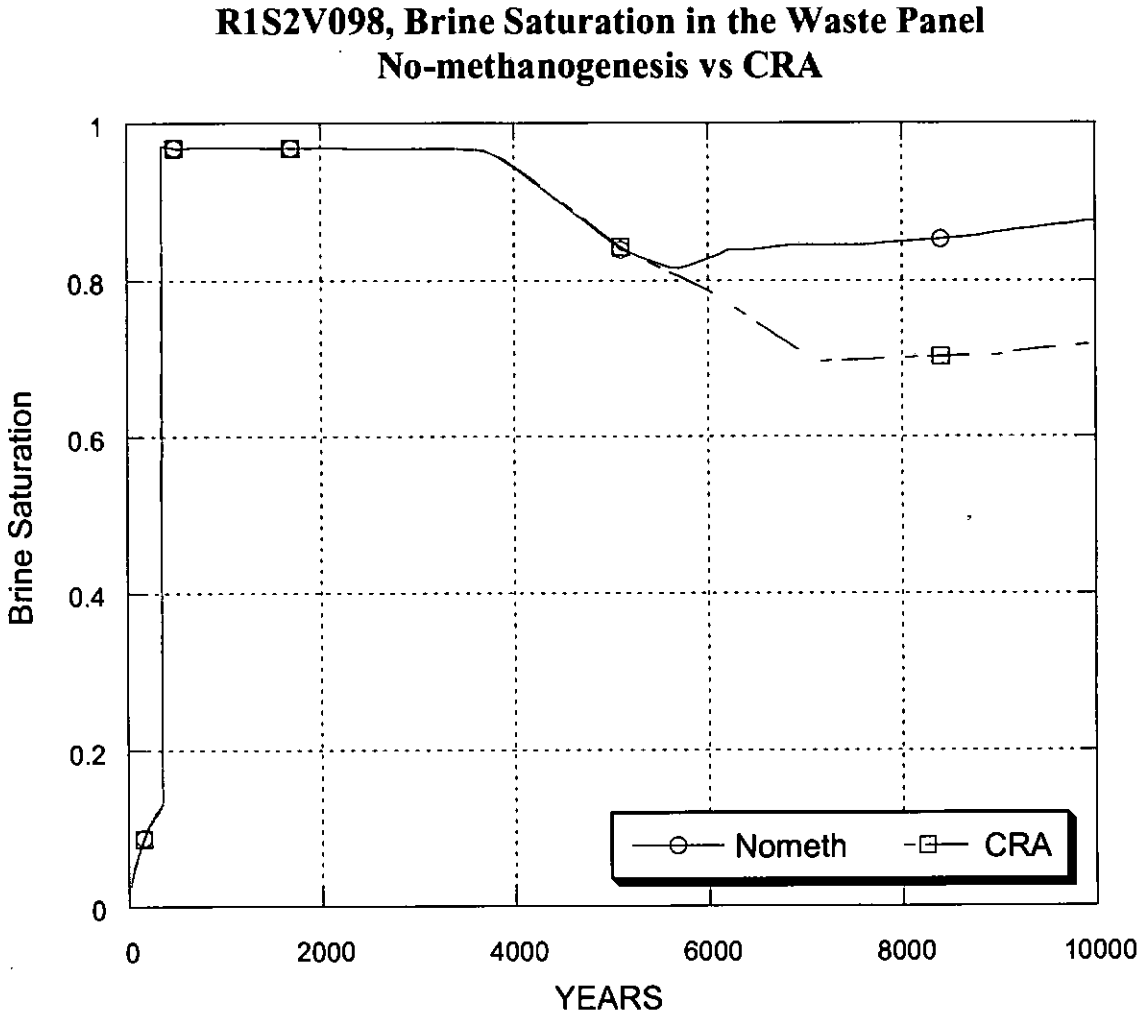

Figure 7. Brine saturation in the waste panel for vector 98 in scenario S2. Here red points (lines) are results without methanogenesis, and blue represents results from the CRA. The times plotted are listed in Table 2.

all six scenarios of the CRA (Stein and Zelinski, 2003). Vector 98 in scenario S2 of the no-methanogenesis calculations required only one convergence adjustment. Thus we believe that the anomalous results of vector 98 occurred due to relaxed convergence parameters. However this result had no discernable effect on brine saturation statistics for the waste panel (Figure 9). As with pressure, small differences in brine saturation for individual vectors over limited time ranges do not effect the statistical distribution of brine saturation values in the waste panel for either scenario (Figures 8 and 9).

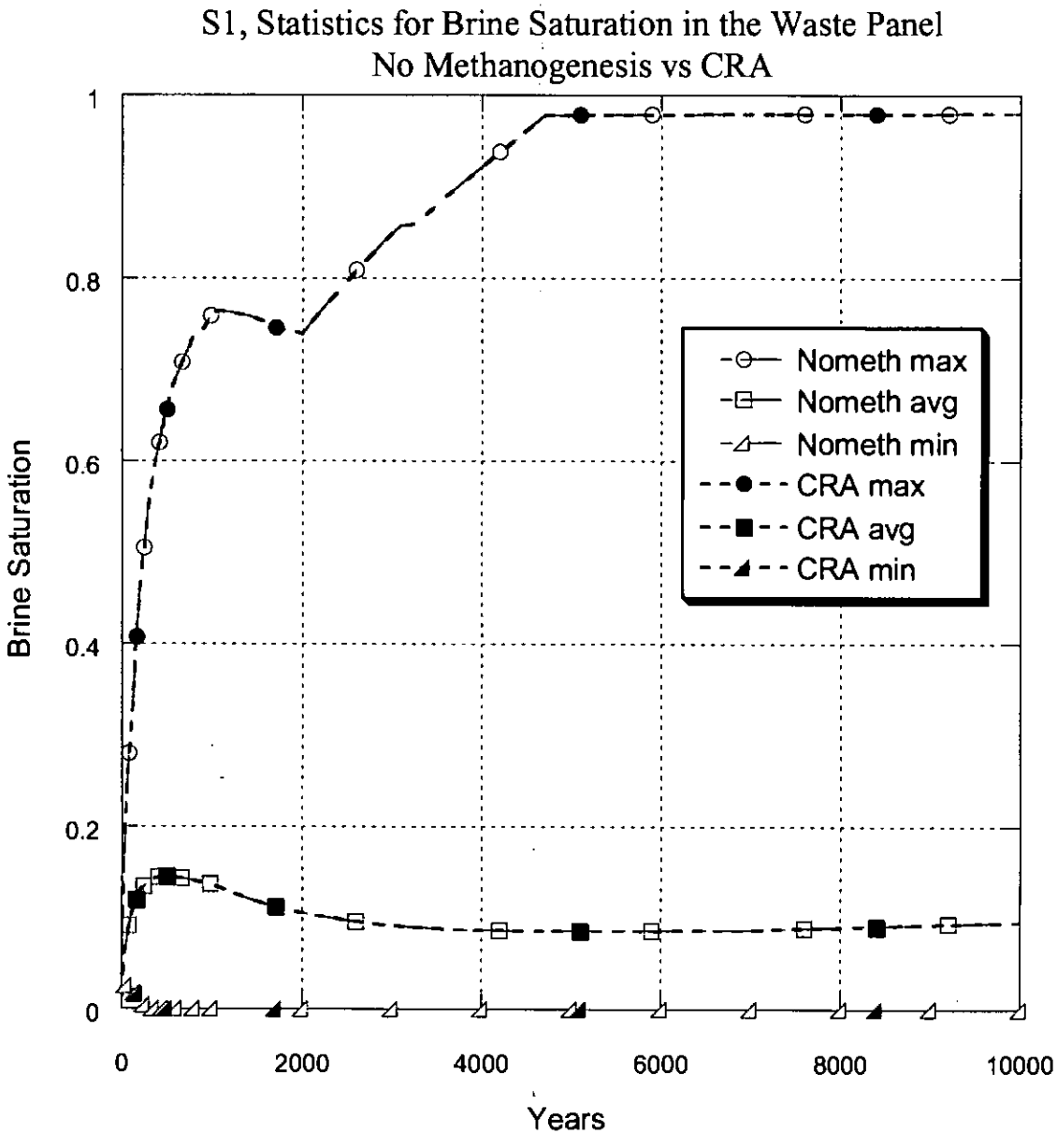

Figure 8. Brine saturation in the waste panel from scenario S1. Red points and lines represent results without methanogenesis. Black points (lines) represent results from the CRA. The maximum curve is the maximum over all vectors at each time plotted, same for the average and the minimum. The times plotted are listed in Table 2.

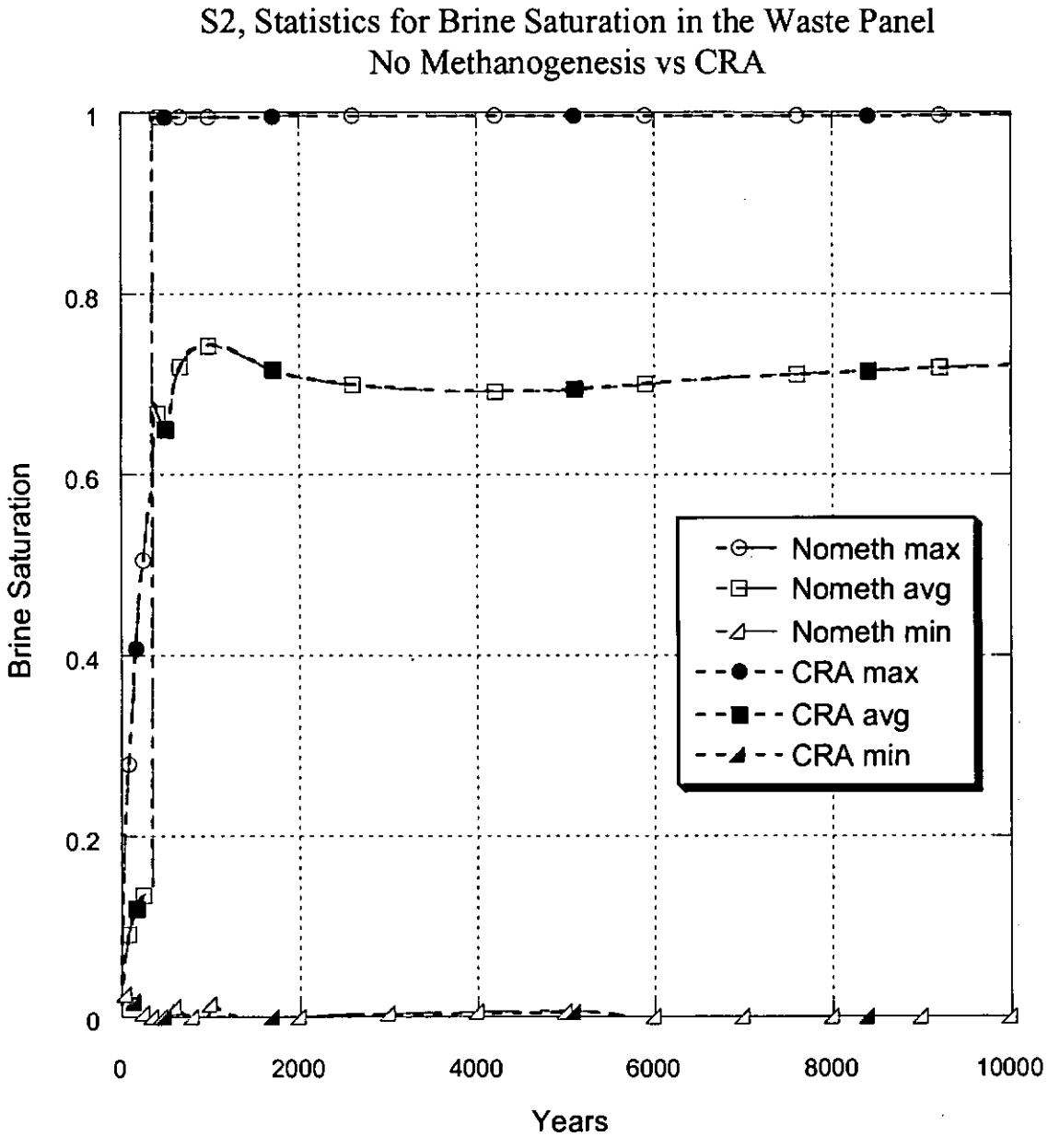

Figure 9. Brine saturation in the waste panel in scenario S2. Points and colors are the same as Figure 8.

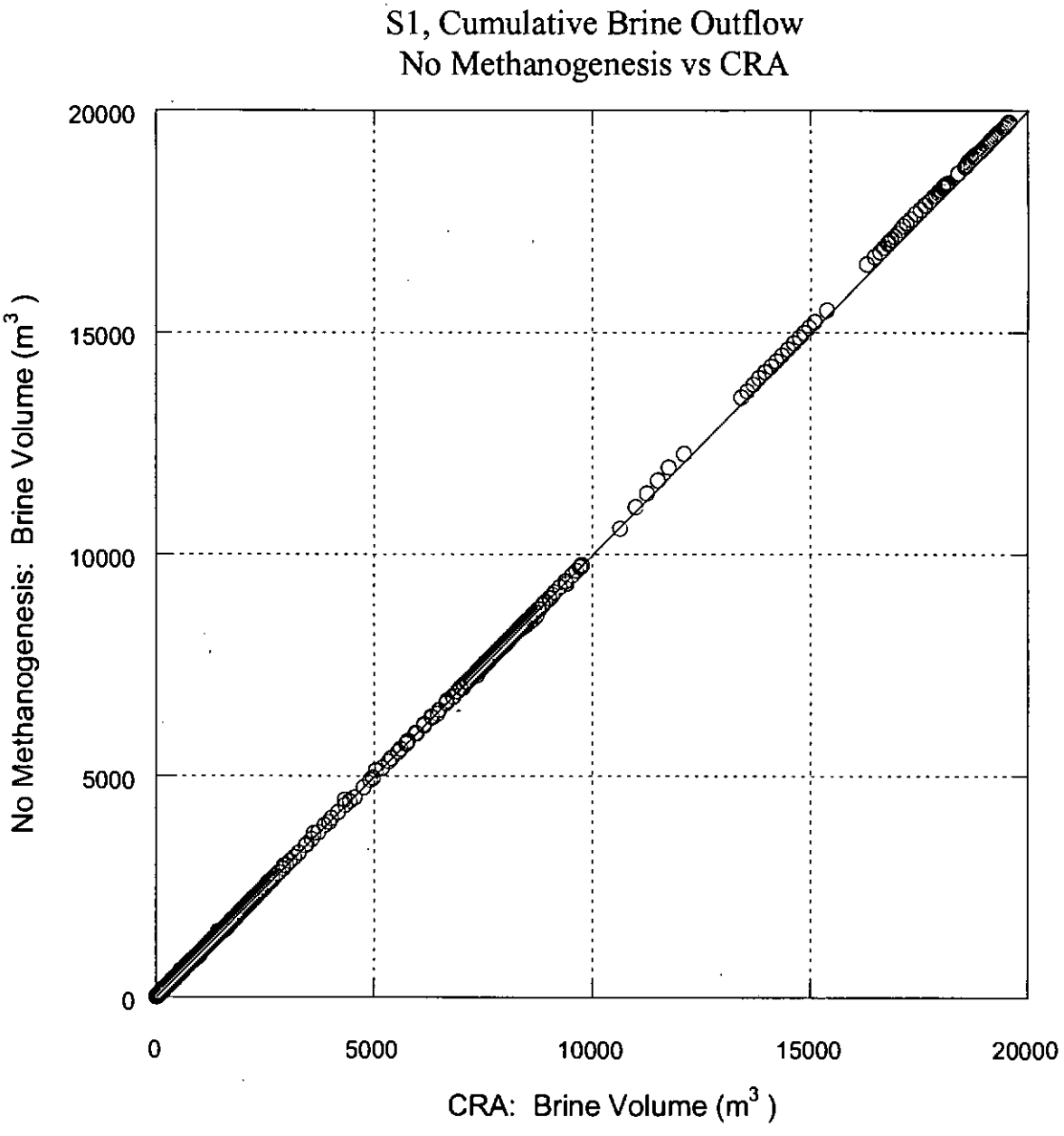

Figure 10. Scatter plot of cumulative brine outflow in scenario S1. Points are cumulative brine outflow from each vector, without methanogenesis versus that obtained from CRA calculations. The times plotted are listed in Table 2.

5.3 Brine Outflow

Figures 10-11 present scatter plots of cumulative brine outflow (BRINREPOC) for the no-methanogenesis calculations versus the CRA. The point pairs for both scenario S1 and S2 comprise virtually straight lines. Brine outflow is very slightly increased with no-methanogenesis in a few vectors that had the highest brine outflow in the CRA, but the differences are inconsequential to repository performance.

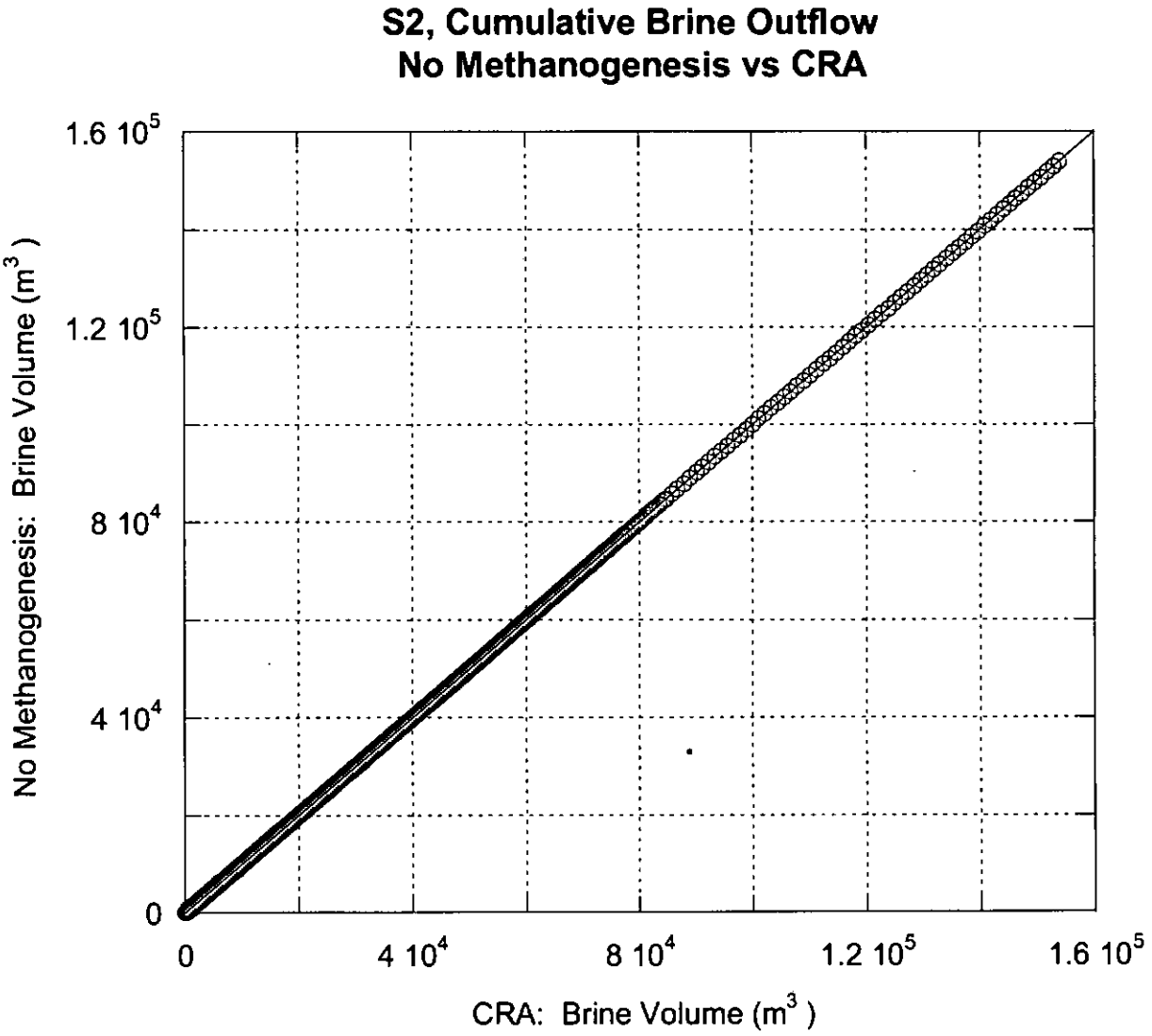

Figure 11. Scatter plot of cumulative brine outflow for scenario S2. Points have the same meaning as in Figure 10.

As with pressure and brine saturation, the statistical distribution of brine outflow values over 100 vectors is not visually noticeable over the entire 10,000-year modeling period (Figures 12-13).

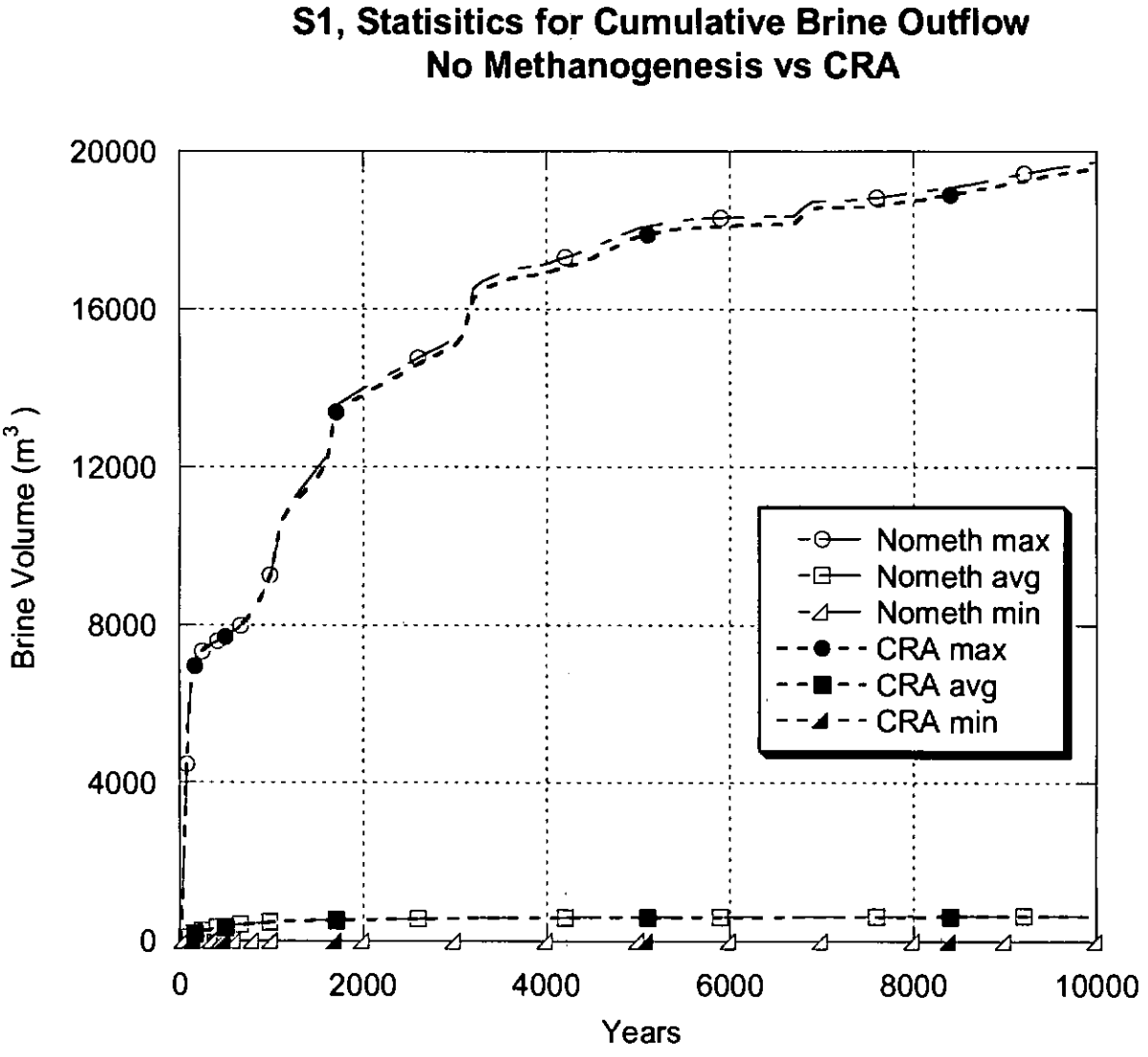

Figure 12. Cumulative brine outflow versus time for scenario S1. Red points and lines represent results without methanogenesis. Black points (lines) represent results from the CRA. The maximum brine outflow curve is the maximum over all vectors at each time plotted, same for the avg and the min. The times plotted are listed in Table 2.

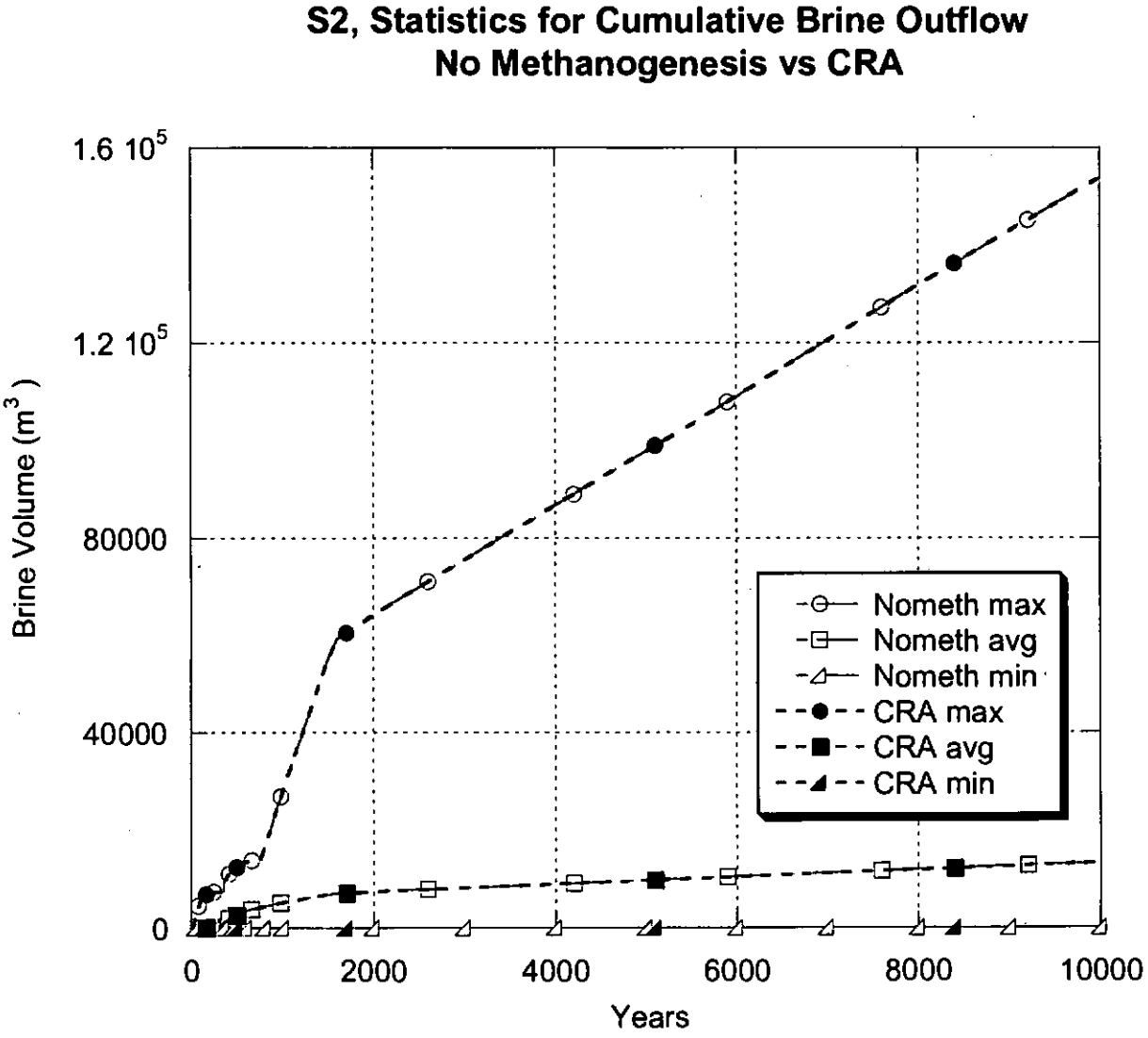

Figure 13. Cumulative Brine Outflow versus time for scenario S2. Points colors and lines have the same meaning as in Figure 12.

6 RUN CONTROL • CALCULATIONS FOR REMOVAL OF METHANOGENESIS

Digital Command Language (DCL) scripts, referred to here as EVAL run scripts, are used to implement and document the running of all software codes. These scripts, which are the basis for the WIPP PA run control system, are stored in the CRA1_EVAL CMS library. All inputs are fetched at run time by the scripts, and outputs and run logs are automatically stored by the scripts in class CRA1 of the CMS libraries.

Table 3. BRAGFLO Run Control Files: Step 1

Code	Filename	File Type	CMS LIBRARY, location	comments, > **USED BY**, < FROM
Script	EVAL_BF_CRA1V_RUN.COM	script	CRA1V_EVAL	instance script
	EVAL_BF_CRA1V_RUN_MASTER.COM	script	CRA1V_EVAL	distribution script
	EVAL_BF_CRA1V_STEP1.INP	script	CRA1V_EVAL	script input file
	BF_CRA1V_R*x*_S*y*_STEP1.LOG	output	CRA1V_BFRxSy	script log file
GENMESH	gm_PA96.exe	executable	wp$prodroot:[gm.exe]	run for each R (1)
	GM_BF_CRA1V.INP	input	CRA1V_GM	provided by JSSTEIN
	GM_BF_CRA1V.CDB	output	CRA1V_GM	> **MATSET**
	GM_BF_CRA1V.DBG	output	temporary (wd)	
MATSET	matset_qa0910.exe	executable	wp$prodroot:[ms.exe]	run for each R (1)
	MS_BF_CRA1V.INP	input	CRA1V_MS	provided by WPZELIN
	GM_BF_CRA1V.CDB	input	CRA1V_GM (wd)	< GENMESH
	MS_BF_CRA1V.CDB	output	CRA1V_MS	> **POSTLHS**
	MS_DBG$OUTPUT.DAT	output	temporary (wd)	
PRELHS	prelhs_qa0230.exe	executable	wp$prodroot:[lhs.exe]	run for each R (1)
	LHS1_BF_CRA1V_A*x*.INP	input	CRA1V_LHS	provided by WPZELIN
	LHS1_BF_CRA1V_TRN_A*x*.OUT	output	CRA1V_LHS	> **LHS**
	LHS1_BF_CRA1V_A*x*.OUT	output	CRA1V_LHS	
LHS	lhs_PA96.exe	executable	wp$prodroot:[lhs.exe]	run for each R (1)
	LHS1_BF_CRA1V_TRN_A*x*.OUT	input	CRA1V_LHS (wd)	< PRELHS
	LHS2_BF_CRA1V_TRN_A*x*.OUT	output	CRA1V_LHS	> **POSTLHS**
	LHS2_BF_CRA1V_DBG_A*x*.OUT	output	CRA1V_LHS	

Code	Filename	File Type	CMS LIBRARY, location	comments, > **USED BY**, < FROM
POSTLHS	postlhs_PA96.exe	executable	wp$prodroot:[lhs.exe]	run for each R (1)
	MS_BF_CRA1V.CDB	input	CRA1V_MS (wd)	< MATSET
	LHS2_BF_CRA1V_TRN_A*x*.OUT	input	CRA1V_LHS (wd)	< LHS
	LHS3_BF_CRA1V.INP	input	CRA1V_LHS	dummy file required by LHS3
	LHS3_BF_CRA1V_A*x*_R*nnn*.CDB	output	CRA1V_LHS	**> ICSET**
	LHS3_BF_CRA1V_A*x*.DBG	output	temporary (wd)	
	LHS3_BF_CRA1V_A*x*1.SCR	scratch	temporary (wd)	opened, used, closed, deleted
	LHS3_BF_CRA1V_A*x*2.SCR	scratch	temporary (wd)	opened, used, closed, deleted
ICSET	icset_PA96.exe	executable	wp$prodroot:[ic.exe]	run for each R (1), V (100)
	LHS3_BF_CRA1V_A*x*_R*nnn*.CDB	input	CRA1V_LHS (wd)	< POSTLHS
	IC_BF_CRA1V.INP	input	CRA1V_IC	provided by WPZELIN
	IC_BF_CRA1V_R*x*_V*nnn*.CDB	output	temporary (wd)	**> ALGEBRACDB**
	IC_BF_CRA1V_R*x*_V*nnn*.DBG	output	temporary (wd)	
ALGEBRACDB	algebracdb_PA96.exe	executable	wp$prodroot:[alg.exe]	run for each R (1), V (100)
	IC_BF_CRA1V_R*x*_V*nnn*.CDB	input	working_dir	< ICSET
	ALG1_BF_POSTCRA.INP	input	CRA1V_ALG	provided by MBNEMER
	ALG1_BF_CRA1V_R*x*_V*nnn*.CDB	output	CRA1V_ALG	**> PREBRAG, > POSTBRAG**
	ALG1_BF_CRA1V_R*x*_V*nnn*.DBG	output	temporary (wd)	

Table 4. BRAGFLO Run Control Files: Step 2

Code	Filename	File Type	CMS LIBRARY, location	comments, > **USED BY**, < FROM
Script	EVAL_BF_CRA1V_RUN.COM	script	CRA1V_EVAL	instance script
	EVAL_BF_CRA1V_RUN_MASTER.COM	script	CRA1V_EVAL	distribution script
	EVAL_BF_CRA1V_STEP2.INP	script	CRA1V_EVAL	script input file
	BF_CRA1V_R*x*S*y*V*nnn*STEP2.LOG	output	CRA1V_BFRxSy	script log file
PREBRAG	prebrag_qb0700.exe	executable	wp$prodroot:[bf.exe]	run for each R (1), S (2), V (100)
	BF1_CRA1V_S*y*.INP	input	CRA1V_BF	provided by WPZELIN
	ALG1_BF_CRA1V_R*x*_V*nnn*.CDB	input	CRA1V_ALG	< ALGEBRACDB
	BF1_CRA1V_R*x*_S*y*_V*nnn*.DBG	output	temporary (wd)	
	BF2_CRA1V_R*x*_S*y*_V*nnn*.INP	output	CRA1V_BFRxSy	**> BRAGFLO**

Run for each replicate (R1), scenario (S1–S2), and vector (V001–V100) = 200 runs.
CMS class = CH4

Table 5. BRAGFLO Run Control Files: Step 3.

Code	Filename	File Type	CMS LIBRARY, location	comments, > **USED BY**, < FROM
Script	EVAL_BF_CRA1V_RUN.COM	script	CRA1V_EVAL	instance script
	EVAL_BF_CRA1V_RUN_MASTER.COM	script	CRA1V_EVAL	distribution script
	EVAL_BF_CRA1V_STEP3.INP	script	CRA1V_EVAL	script input file
	BF_CRA1V_R*x*S*y*V*nnn*_STEP3.LOG	output	CRA1V_BFRxSy	script log file
BRAGFLO	bragflo_qa0500.exe	executable	wp$prodroot:[bf.exe]	run for each R (1), S (2), V (100)
	BF2_CRA1V_R*x*_S*y*_V*nnn*.INP	input	CRA1V_BFRxSy (ws)	< PREBRAG
	BF2_CRA1V_CLOSURE.DAT	input	CRA1V_BF	provided by WPZELIN
	BF2_CRA1V_R*x*_S*y*_V*nnn*.OUT	output	temporary (wd)	
	BF2_CRA1V_R*x*_S*y*_V*nnn*.SUM	output	temporary (wd)	
	BF2_CRA1V_R*x*_S*y*_V*nnn*.BIN	output	temporary (wd)	**> POSTBRAG**
	BF2_CRA1V_R*x*_S*y*_V*nnn*.ROT	output	temporary (wd)	
	BF2_CRA1V_R*x*_S*y*_V*nnn*.RIN	output	temporary (wd)	
POSTBRAG	postbrag_PA96.exe	executable	wp$prodroot:[bf.exe]	run for each R (1), S (2), V (100)
	BF2_CRA1V_R*x*_S*y*_V*nnn*.BIN	input	working_dir	< BRAGFLO
	ALG1_BF_CRA1V_R*x*_V*nnn*.CDB	input	CRA1V_ALG (wd)	< ALGEBRACDB
	BF3_CRA1V_R*x*_S*y*_V*nnn*.CDB	output	CRA1V_BFRxSy	**> ALGEBRACDB_2**
	BF3_CRA1V_R*x*_S*y*_V*nnn*.DBG	output	temporary (wd)	

Run for each replicate (R1), scenario (S1–S2), and vector (V001–V100) = 200 runs.
CMS class = CH4

Table 6. BRAGFLO Run Control Files: Step 3 Exception Vectors.

Code	Filename	File Type	CMS LIBRARY, location	comments, > USED BY, < FROM
Script	EVAL_BF_CRA1V_RUN.COM	script	CRA1V_EVAL	instance script
	EVAL_BF_CRA1V_RUN_MASTER.COM	script	CRA1V_EVAL	distribution script
	EVAL_BF_CRA1V_STEP4.INP	script	CRA1V_EVAL	script input file
	BF_CRA1V_R*x*S*y*V*nnn*_STEP4.LOG	output	CRA1V_BFRxSy	script log file
ALGEBRACDB_2	algebracdb_PA96.exe	executable	wp$prodroot:[alg.exe]	run for each R (1), S (2), V (100)
(aka POSTALG)	BF3_CRA1V_R*x*_S*y*_V*nnn*.CDB	input	CRA1V_BFRxSy (ad)	< POSTBRAG
	ALG2_BF_POSTCRA.INP	input	CRA1V_ALG	provided by WPZELIN
	ALG2_CRA1V_R*x*_S*y*_V*nnn*.CDB	output	CRA1V_BFRxSy	
	ALG2_BF_CRA1V_R*x*S*y*V*nnn*.DBG	output	temporary (wd)	

Run for each replicate (R1), scenario (S1–S2), and vector (V001–V100) = 200 runs.
CMS class = CH4

Table 7. BRAGFLO Run Control Files: Step 3 Exception Runs.

Code	Filename	File Type	CMS LIBRARY, location	comments, > USED BY, < FROM
Script	EVAL_BF_CRA1V_RUN.COM	script	CRA1V_EVAL	instance script
	EVAL_BF_CRA1V_RUN_MASTER.COM	script	CRA1V_EVAL	distribution script
	EVAL_BF_CRA1V_STEP3_MOD.INP	script	CRA1V_EVAL	script input file
	BF_CRA1V_R*x*S*y*V*nnn*_STEP3.LOG	output	CRA1V_BFRxSy	script log file
BRAGFLO	Same as BRAGFLO Step 3 above except for MOD files which are modified input files			
	BF2_CRA1V_R*x*_S*y*_V*nnn*_MOD.INP	input	CRA1V_BFRxSy	provided by WPZELIN
POSTBRAG	Same as BRAGFLO Step 3 above			

Run for vectors R1S1V098, R1S2V079, R1S2V098 = 3 runs.
CMS class = CH4

The preceding tables constitute the run control documentation for the removal of methanogenesis calculations. Each table is labeled with the main code, and process step (if applicable). Many code sets are broken down into a first step (step 1) which runs utility codes such as Genmesh (GM), Matset (MS), LHS, etc., and subsequent steps (step 2, ...) which run the primary code along with any pre and post processors. Step 1 codes are generally run once, or once per replicate, while step 2 codes are generally run once per vector.

Run control tables are intended to provide all the information required to document a calculation. The tables contain five columns:

Code — the descriptive common code name (ICSET, ALGEBRACDB, BRAGFLO, etc.) indicating the row relates to that code, "Script" indicating the row relates to the run control system, or blank indicating the row relates to the previous code label. Completely blank rows are for visual separation only.

Filename — VMS filename in the form <filename>.<extension>. Placeholders are included when multiple replicates, scenarios, vectors, cavities, time intrusions, ... are being represented (see footnote below).

File Type — the type of file being identified from the point of view of the current step of the run control system. These include script, executable, input, output, and scratch. Note that the output of one step may become the input of an ensuing step.

CMS LIBRARY, location — the CMS library where the controlled version of the file can be found, "temporary (wd)" indicating the file is not stored in CMS (many files generated by a calculation are for debug purposes, or are intermediate in nature, and are not retained after execution), "(wd)" or "(ad)" following a CMS library name indicating the input, though stored in CMS, is pulled from the temporary working directory or analysis directory (respectively) for convenience, "working_dir" indicating the input is from a temporary file produced by an earlier code, or other lowercase strings indicating the VMS directory pathname where the file (generally an executable) is located.

comments, > **USED BY**, < FROM — comments typed in lowercase, a bold greater than sign (>) followed by a bold code name indicating the output file is used as input for the specified code, a less than sign (<) followed by a code name indicating the input file was generated as output by the specified code.

The replicate, scenario, vector, etc. numbers shown below the label of each table indicate the *actual* runs. The numbers in parentheses shown in the comment field of each executable indicate the *count* of replicates, scenarios, vectors, etc. For example, if a certain calculation were run on R3, S4–6, V051–V100, then the comment would show R (1), S (3), V (50) indicating a total of 150 runs.

In Table 3-Table 7:

- R*x*—used to denote multiple replicates, where x = 1–3. Seen as A*x* in LHS
- S*y*—used to denote multiple scenarios, where y = 1–6
- V*nnn*—used to denote multiple vectors, where *nnn* = 1–100. Seen as R*nnn* in LHS
- (wd)—working_dir
- (ad)—analysis_dir

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