Development and Application of an Analysis Methodology for Interpreting Ambiguous Historical Pressure Data in the WIPP Gas-Generation Experiments

**prepared by
Engineering Technology Division
Argonne National Laboratory-West**

NT Technical Memorandum

Results reported in the NT-TM series of memoranda frequently are preliminary and subject to revision. Consequently, they should not be quoted or referenced.

**Argonne National Laboratory is managed by
The University of Chicago for the U. S. Department of Energy**

About Argonne National Laboratory

Argonne is managed by The University of Chicago for the U.S. Department of Energy under contract W-31-109-Eng-38. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne and its pioneering science and technology programs, see www.anl.gov.

Availability of This Report

This report is available, at no cost, at <http://www.osti.gov/bridge>. It is also available on paper to U.S. Department of Energy and its contractors, for a processing fee, from:

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
phone (865) 576-8401
fax (865) 576-5728
reports@adonis.osti.gov

Disclaimer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor The University of Chicago, nor any of their employees or officers, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of document authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof, Argonne National Laboratory, or The University of Chicago.

Development and Application of an Analysis Methodology for Interpreting Ambiguous Historical Pressure Data in the WIPP Gas-Generation Experiments

by

F.S. Felicione*

Engineering Technology Division, Argonne National Laboratory-West

*Current Affiliation: Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415

THE UNIVERSITY OF
CHICAGO

Argonne National Laboratory is managed by
The University of Chicago for the U.S. Department of Energy

TABLE OF CONTENTS

	<u>Page</u>
ACRONYMS.....	viii
NOMENCLATURE.....	ix
SUBSCRIPTS	x
GREEK SYMBOLS	xi
ABSTRACT.....	xiii
1.0 Introduction and Summary	1
1.1 Gas-Generation Experiments and Task Background	1
1.2 Operational Experience with the GGE	3
1.3 Initial Data Analyses.....	3
1.4 Approach and Objectives of the Present Investigation	5
1.4.1 Validation of the Test Data.....	5
1.4.2 Recovery of the Archived Pressure Data.....	6
1.5 Organization of the Report.....	6
2.0 GGE Experiment Configuration	7
2.1 Test Container Description	7
2.2 Glovebox.....	9
3.0 Overview of the Measured Data	12
4.0 Analysis Development.....	13
4.1 Application of the State Equation.....	13
4.2 Analysis Approach.....	15
5.0 Headspace-Gas-Mass Considerations.....	15
5.1 Headspace-Gas Composition and Volatility	15
5.2 Sources of Variation in the Headspace-Gas Mass	17
5.2.1 Discrete Headspace-Gas-Mass Variation.....	17
5.2.2 Continuous Headspace-Gas-Mass Variation.....	19
5.2.3 Gas-Solubility Variation	20
5.3 Gas-Generation-Rate Specification	21
5.3.1 Increase in Headspace-Gas Mass by Gas Generation.....	21
5.3.2 Mole Fraction of Generated Gases	23
5.3.3 Rates of Gas Generation	23
6.0 Headspace Volume Considerations.....	24
6.1 Headspace Volume Variation	24
6.1.1 Test-Container Expansion/Contraction.....	25
6.1.2 Expansion/Contraction in the Brine and Waste	26
6.2 Headspace Volume Determination.....	26
6.2.1 Headspace-Gas Expansion Measurements	27

TABLE OF CONTENTS (Contd.)

	<u>Page</u>
6.2.2 Adjustment of the Headspace Volume Measurements.....	29
7.0 Headspace-Gas Compressibility	31
8.0 Headspace-Gas Temperatures	33
8.1 Equilibrium Temperatures	33
8.2 Mechanical Generation of Heat	41
9.0 Validation of the GGE Data	44
9.1 Computation at a Specific Point	44
9.1.1 Temperature Ratio	44
9.1.2 Compressibility Ratio	45
9.1.3 Mass Ratio	45
9.1.4 Headspace-Volume Ratio	46
9.1.5 Predicted Pressure	48
9.1.6 Compensated Pressure	49
9.1.7 Mechanical Work	49
9.2 Adjustment of the Pressures in the Blank, Experiment-Control Test Containers.....	50
10. Recovery of the Archived Pressure Measurements	55
10.1 Determination of the Brine/Waste Thermal Expansion Coefficient	55
10.2 Instrument Calibrations.....	60
11. Recovered Data	60
11.1 Analysis Results.....	60
11.2 Discussion	79
11.2.1 Adjusted Pressure Results.....	79
11.2.2 Examination for Evidence of Gas Generation	82
12.0 Applicability to Other Investigations and Experiment-Design Implications.....	84
12.1 Pressure Sensitivity to Operating Pressure	85
12.2 Pressure Sensitivity to Headspace/Waste Volume Ratio.....	85
12.3 Comparison of the GGE to Other Gas-Generation Experiments.....	85
13.0 Limitations of the Analyses	86
REFERENCES	89
ACKNOWLEDGEMENT	90
APPENDIX A. Gas-Solubility Variation.....	91
A1. Diffusion Model.....	91
A2. Diffusion/Convection Model	93
APPENDIX B. Thermal Expansion Experiments	99

TABLE OF CONTENTS (Contd.)

	<u>Page</u>
APPENDIX B ATTACHMENT	105
APPENDIX C. Local Glovebox Temperature Determination.....	109
C1. Temperature Mapping.....	109
C2. Excess-Temperature Algorithm	109
APPENDIX C ATTACHMENT	111
APPENDIX D. Computer Application Program	115
D1. Program Input	115
D2. Specification of the Test Container to be Analyzed.....	116
D3. Program Output.....	116
D4. Program Map and Listing	116
D5. Execution of the Program	116
D6. Results Plots.....	117
APPENDIX D ATTACHMENTS.....	118

LIST OF FIGURES

	<u>Page</u>
1. Temperature Trace for a Step Increase in the Heater Setpoint	4
2. Pressure Trace for a Step Increase in the Heater Setpoint	5
3. Test Container Vertical Section	8
4. Test-Container Shroud and Heater-Band Arrangement	9
5. Assembled Test Container	10
6. Assembled Test Container in Glovebox with Instrumentation Connections	11
7. GGE Glovebox Configuration	11
8. Test Container and Glovebox Temperatures for a Typical Test Container	12
9. Synchronization of Test Container Pressure with Temperature	13
10. Representation of Discrete Events at Times Prior To and Beyond the Reference Point	18
11. Depiction of the Headspace Volume Measurement	27
12. Compressibility Factor for Nitrogen Gas	31
13. Discretization for the Two-Dimensional Thermal Model	34
14. One-Dimensional Thermal Model	36
15. Hypothesized Axial Temperature Distribution in the Brine/Waste	38
16. Two-Dimensional Effects in the Test-Container Head Region	38
17. Mechanical Work of Compression in the Headspace Gas	42
18. Temperatures, TC-152	52
19. Temperatures, TC-153	52
20. Pressures, TC-152	53
21. Pressures, TC-153	53
22. Gas Generation in TC-152	54
23. Gas Generation, TC-153	55
24A. Temperatures, TC-151	61
24B. Pressures, TC-151	62
24C. Gas Generation in TC-151	62
25A. Temperatures, TC-160	63
25B. Pressures, TC-160	63
25C. Gas Generation in TC-160	64
26A. Temperature, TC-161	64
26B. Pressures, TC-161	65
26C. Gas Generation in TC-161	65
27A. Temperatures, TC-162	66
27B. Pressures, TC-162	66
27C. Gas Generation in TC-162	67
28A. Temperatures, TC-163	67
28B. Pressures, TC-163	68

LIST OF FIGURES (Contd.)

	<u>Page</u>
28C. Generated Gas, TC-163	68
29A. Temperature, TC-164	69
29B. Pressure, TC-164	69
29C. Gas Generation in TC-164	70
30A. Temperatures, TC-165	70
30B. Pressures, TC-165	71
30C. Gas Generation, TC-165	71
31A. Temperatures, TC-166	72
31B. Pressures, TC-166	72
31C. Gas Generation, TC-166	73
32A. Temperatures, TC-167	73
32B. Pressures, TC-167	74
32C. Gas Generation, TC-167	74
33A. Temperatures, TC-168	75
33B. Pressures, TC-168	75
33C. Gas Generation, TC-168	76
34A. Temperatures, TC-169	76
34B. Pressures, TC-169	77
34C. Gas Generation, TC-169	77
35A. Temperatures, TC-170	78
35B. Pressures, TC-170	78
35C. Gas Generation, TC-170	79
36. Temperatures, TC-161 - Empirical RTD-Calibration Corrections	80
37. Pressures, TC-161 - Empirical RTD-Calibration Corrections	81
38. Gas Generation in TC-161 - Empirical RTD Calibration Corrections	81
A1. Diffusion Model for Headspace-Gas Solubility	91
A2. Solution to the Pure Diffusion Model	93
A3. Heat-Conduction and Convection Model for Determining the Temperature	94
A4. Enhancement to the Thermal Conductivity to Account for Natural Convection	95
A5. Diffusion/Convection Model for Gas Solubility in the Brine	96
B1. Experiment Configuration for Determination of the Volumetric, Thermal-Expansion Coefficients for Pure Water and Brine	99
B2. Experiment Apparatus for Determination of the Volumetric, Thermal-Expansion Coefficient	100
B3. Test Vessel for the Thermal-Expansion Measurements	101
B4. Top View of the Test Vessel in its Water Bath	102
B5. Measured Volumetric Coefficients of Thermal-Expansion for Pure Water	103
B6. Measured Volumetric Coefficients of Thermal-Expansion for Brine A	103
C1. Estimate of Local Test Container Temperature Excess	110

LIST OF TABLES

	<u>Page</u>
1. Waste Contents Within Each Test Container	1
2. Best Estimate Headspace Volumes at the Reference Conditions	30
3. Thermo-Physical Properties Used in the Thermal Model	40
4. Raw Headspace Volume Measurements for TC-153	46
5. Adjusted Headspace Volume Measurements for TC-153	47
6. Volumetric Coefficients of Thermal Expansion in the Brine/Waste	59
7. Comparison of RTD Calibration Corrections for TC-161: Recorded versus Empirical Corrections	82
8. Graphically Inferred Gas-Generation Rates	83

ACRONYMS

AISI	American Iron and Steel Institute
ANL-West	Argonne National Laboratory - West
DOE	[U.S.] Department of Energy
GGE	Gas-Generation Experiments
ID	Internal diameter
PID	Proportional, integral, and derivative [controller]
PXD	Pressure transducer
RTD	Resistance temperature detector
SNL	Sandia National Laboratory
TRU	Transuranic
UNS	Unified Number System
WIPP	Waste Isolation Pilot Plant
ZPPR	Zero Power Physics Reactor

NOMENCLATURE

A	Constant defined by Equations 7-2 and 7-3
a	Constant defined by Equations 7-2 and 7-3
B	Constant defined by Equations 7-2 and 7-3
b	Constant defined by Equations 7-2 and 7-3
c	Constant defined by Equations 7-2 and 7-3
c_v	Specific heat capacity at constant volume
e	Constant defined by Equations 7-2 and 7-3
h	Heat-transfer coefficient or conductance value
[MW]	Molecular weight
M	Mass
N	Moles
P	Pressure
Q	Heat transfer to the headspace gas
q	Heat flux
R	Gas constant (mass specific)
R_U	Gas constant (mole specific)
s	Entropy
T	Temperature
t	Time
U	Internal energy
V	Volume
v	Specific volume
W	Work performed by the headspace gas on the brine/waste
X	Mole fraction of dissolved gas when the gas pressure equals one atmosphere

x	Mole fraction of dissolved gas with any gas pressure
z	Compressibility factor

SUBSCRIPTS

adj	Adjusted value
ave	Arithmetic average
c	Container
cal	Calibration value
calc	Calculated value
comp	Compensated value
corr	Amount of correction
D	Denotes a discrete event
dis	Dissolved quantity
GB	Glovebox
g	Gas (in the headspace)
gen	Result of gas generation
H	High value for β determination
HS	Headspace
L	Low value for β determination
l	Liquid (brine)
ME	Mechanical energy
RTD	Measurement by the resistance temperature detector in the brine or glovebox
sampling	Resulting from sample extraction

sol	Resulting from solubility variation
PXD	Pressure transducer calibration
s	Sample
step	Resulting from a step change in the test container temperature
v	Vapor
0	Initial condition or reference value
1	Region defined in the thermal model
2	Region defined in the thermal model
3	Region defined in the thermal model
∞	Region defined in the thermal model

GREEK SYMBOLS

α	Linear coefficient of thermal expansion
β	Volumetric coefficient of thermal expansion
Δ	Difference
δ	Small difference
γ	Ratio of the heat capacity at constant pressure to the heat capacity at constant volume

DEVELOPMENT AND APPLICATION OF AN ANALYSIS METHODOLOGY FOR INTERPRETING AMBIGUOUS HISTORICAL PRESSURE DATA IN THE WIPP GAS-GENERATION EXPERIMENTS

by

F. S. Felicione

ABSTRACT

The potential for generation of gases in transuranic (TRU) waste by microbial activity, chemical interactions, corrosion, and radiolysis was addressed in the Argonne National Laboratory-West (ANL-West) Gas-Generation Experiments (GGE). Data was collected over several years by simulating the conditions in the Waste Isolation Pilot Plant (WIPP) after the eventual intrusion of brine into the repository. Fourteen test containers with various actual TRU waste immersed in representative brine were inoculated with WIPP-relevant microbes, pressurized with inert gases, and kept in an inert-atmosphere environment for several years to provide estimates of the gas-generation rates that will be used in computer models for future WIPP Performance Assessments.

Modest temperature variations occurred during the long-term ANL-West experiments. Although the experiment temperatures always remained well within the experiment specifications, the small temperature variation was observed to affect the test container pressure far more than had been anticipated. In fact, the pressure variations were so large, and seemingly erratic, that it was impossible to discern whether the data was even valid and whether the long-term pressure trend was increasing, decreasing, or constant. The result was that no useful estimates of gas-generation rates could be deduced from the pressure data. Several initial attempts were made to quantify the pressure fluctuations by relating these to the measured temperature variation, but none was successful.

The work reported here carefully analyzed the pressure measurements to determine if these were valid or erroneous data. It was found that a thorough consideration of the physical phenomena that were occurring can, in conjunction with suitable gas laws, account quite accurately for the pressure changes that were observed. Failure of the earlier attempts to validate the data was traced to the omission of several phenomena, the most important being the variation in the headspace volume caused by thermal expansion and contraction within the brine and waste.

A further effort was directed at recovering useful results from the voluminous archived pressure data. An analytic methodology to do this was developed. This methodology was applied to each archived pressure measurement to nullify temperature and other effects to yield an adjusted pressure, from which gas-generation rates could be calculated.

A review of the adjusted-pressure data indicated that generated-gas concentrations among these containers after approximately 3.25 years of test operation ranged from zero to over 17,000 ppm by volume. Four test containers experienced significant gas generation. All test containers that showed evidence of significant gas generation contained carbon-steel in the waste, indicating that corrosion was the predominant source of gas generation.

1.0 Introduction and Summary

The long-term performance of the Waste Isolation Pilot Plant (WIPP) in effectively isolating contaminants from the environment is obviously very important to the success of the repository. Sandia National Laboratory (SNL) has the responsibility to make overall performance predictions. These predictions rest on having a good understanding of the behavior of the waste as it interacts with the repository environment, including the potential for migration of contaminants away from the site. A key parameter in these analyses is the predicted rise in repository pressure that may result from gases that are generated in the waste by microbial activity, radiolysis, corrosion, or other chemical reactions following the eventual intrusion of brine into the depository. The resulting increase in the internal pressure in the depository may exceed the lithostatic pressure exerted by the surrounding salt, affecting the calculated rates of migration of contaminants away from the repository. Assumptions made in the formal Performance Assessment calculations that are part of the WIPP licensing process need to be tested to ensure that conservative values were used. The Argonne National Laboratory-West (ANL-West) Gas Generation Experiment (GGE) Program was established to support this work by obtaining accurate data on the rates at which gases are generated in actual radioactive waste at prototypic pressure and temperature.

1.1 Gas-Generation Experiments and Task Background

The GGE was designed to assist SNL in estimating the rates at which gases are produced. The GGE was a very carefully constructed and controlled experiment. Fourteen specially manufactured, corrosion-resistant test containers having a nominal volume of about seven liters each were placed under test. In 12 of these approximately 75% of the container volume was loosely filled with various actual transuranic (TRU) waste. The other two test containers had no wastes and served as experiment controls. A synthetic brine having the same chemical composition as that in the WIPP vicinity was added, filling approximately 90% of the test containers' volumes. To include metabolic gas generation, all containers were inoculated with microbes found at WIPP. These test containers were then backfilled with nitrogen gas and pressurized to approximately 14.87 MPa (2150 psia), the lithostatic pressure level expected to eventually occur at WIPP. Table 1 lists the types of waste materials within each of the test containers.

Table 1. Waste Contents Within Each Test Container

Container Number	Carbon Steel Surface Area (cm ² [in ²])	Aqueous Sludge Mass (g)	Leaded Rubber Mass (g)	Rubber (Neoprene) Mass (g)	Plastic (Polyethylene) Mass (g)	Cloth & Paper (Cellulose) Mass (g)
VSL-151	859.29 (133.19)		129.28			
VSL-152						
VSL-153						

Table 1. (Contd.)

Container Number	Carbon Steel Surface Area (cm ² [in ²])	Aqueous Sludge Mass (g)	Leaded Rubber Mass (g)	Rubber (Neoprene) Mass (g)	Plastic (Polyethylene) Mass (g)	Cloth & Paper (Cellulose) Mass (g)
VSL-160	926.51 (143.61)	269.10	124.72	44.83	91.84	344.24
VSL-161	904.39 (140.18)	273.68	125.96	43.64	86.38	344.35
VSL-162	929.74 (144.11)	267.56	123.36	45.00	86.90	343.85
VSL-163		271.62	125.52			345.22
VSL-164		269.87	127.41			343.72
VSL-165		285.10		43.77	88.47	
VSL-166	902.58 (139.90)	275.63				
VSL-167	905.35 (140.33)			42.52	88.43	345.56
VSL-168						345.90
VSL-169						341.83
VSL-170			123.03	43.48	88.80	

All of the test containers were fitted with highly sensitive and stable temperature and pressure instrumentation, along with suitable systems for periodically extracting very small samples of the vessel headspace gas for chemical analysis. The test containers were placed in an inert-gas (argon)-filled glovebox having a sophisticated gas-purification system to restrict the level of oxygen present. Each test container was fitted with electric heater belts and had its own proportional, integral, and derivative (PID) electronic controller that controlled the temperature of each test container individually to nominally 30°C, the temperature expected in the repository. A data-acquisition system acquired temperature and pressure measurements every hour. Regular calibrations were made to the instruments.

Chemical analyses of the gas samples over the testing period were intended to be used to deduce the rates at which gases were being produced and allow the specific gases generated to be identified. Pressure measurements were to provide a backup indication of gross gas generation. Actual testing began in 1996. By the end of the test program in the Fall, 2002, temperature and pressure data had been collected and archived for over six years, totaling in excess of 50,000 data points per container. (The analysis in this report addresses only the initial 3.25 years of operation, i.e., approximately the first 26,000 hourly data points per test container).

1.2 Operational Experience with the GGE

The GGE tests were conducted within a cell that houses the now-shutdown Zero Power Physics Reactor (ZPPR) at ANL-West. Because of the substantial soil overburden on the reactor cell, the temperature within the reactor cell is relatively cool and tends to remain constant. In combination with the temperature control on each test container, there appeared to be no need to regulate the cell temperature in order to meet the temperature specification of $30 \pm 5^\circ\text{C}$ that was imposed on the experiment. However, since the test containers can be heated, but have no cooling, the local environment needs to be below the 30°C target for the temperature controllers to be active. In fact, the slightly increased temperature within the glovebox that results from the operation of various experiment equipment causes the controllers to become inoperative if the reactor cell temperature exceeds about 28°C .

The reactor cell is air conditioned, and this system can reduce the ZPPR-cell temperature by about 15°C . It was found that long spells of hot summertime weather during the second year of test operation gradually increased the ZPPR-cell temperature above 26°C and required that the air conditioning be used. Temperatures within the test containers, themselves, were nonetheless maintained within a 2-to- 3°C band during all operation of the GGE, in full conformance with the test specifications. Despite the careful design, implementation, and control of the experiments, significant pressure fluctuations were measured. In fact, the fluctuations were so great and so irregular that the validity of the data was questioned, and it was impossible to deduce meaningful pressure trends.

The headspace gas was sampled periodically and analyzed by thermal-conductivity, gas chromatography. Although the gas samples extracted only a few milliliters of headspace gas, pressure decreases of 55-69 kPa (8-10 psi) occurred each time a sample was withdrawn from the small headspace volume (650-750 ml) in each test container. After about one year of operation the puzzling fluctuations in the measured pressure were being recognized. By this time, six or seven headspace-gas samples had been taken from each test container and analyzed. Since each headspace-gas sample degraded the experiment pressure, further sampling was suspended, pending a full explanation of the pressure behavior.

1.3 Initial Data Analyses

Comparisons of the headspace pressure and temperature measurements showed a very obvious *qualitative* correlation in the direction expected: increases or decreases in temperature were consistently accompanied by increases or decreases, respectively, in the measured pressure. Classical gas laws relating pressure and temperature were applied, but these failed to account for even half of the pressure fluctuations measured. As an example, in a particular test container that had been operating at relatively steady conditions the heater set point was deliberately stepped up to a higher setting. The new conditions persisted long enough to allow the test vessel to reach a new steady state, and this caused the temperature to increase in the test container from about 29.6°C to 39.8°C . The event was duly recorded by the data-acquisition system (Fig. 1). A simple ideal-gas pressure-temperature analysis would predict that at the new temperature the pressure should rise from the initial value of 14.615 MPa (2119.7 psia) to a new pressure of

$$P = P_0 \frac{T}{T_0} = 14.615 \text{ MPa} \frac{39.8 + 273.15^\circ \text{C}}{29.6 + 273.15^\circ \text{C}} = 15.107 \text{ MPa} (2191.1 \text{ psia}) \quad (1)$$

Fig. 1. Temperature Trace for a Step Increase in the Heater Setpoint (TC-153)

That is, a pressure rise of about 492.0 kPa (71.4 psi). In fact, the measured pressure rise was actually about 1048.0 kPa (152.0 psi), to 15.663 MPa (2271.7 psia), as shown in Fig. 2, i.e., more than twice as high as the simple pressure-temperature relationship predicts. Application of the pressure-temperature relation to other data points proved equally unable to account for the measured pressure response.

These initial efforts failed to satisfactorily explain, much less quantify, the pressure behavior. Further reviews included attempts to apply empirical correction factors to the data, but with only marginal success, even for the blank, experiment-control containers. Worse still, these empirical approaches emphasized the inability to explain if, and how, the erratic pressure was related to any fundamental phenomenon, calling into question the overall validity of the data. Since the extensive data that had been collected appeared to be of little usefulness, the program sponsor initiated discussions concerning the early termination of the program. Termination of the program would deny the sponsor an important confirmation of assumptions used in the WIPP performance assessment models, as well as deriving no benefit from the considerable investment that had already been made to implement the GGE program. Obviously, early program termination would also eliminate a significant source of on-going funding to ANL-West. The need for a detailed understanding of the pressure fluctuations was clear, and this prompted the rigorous investigation reported here.

Fig. 2. Pressure Trace for a Step Increase in the Heater Setpoint (TC-153)

1.4 Approach and Objectives of the Present Investigation

1.4.1 Validation of the Test Data

The present investigation carefully examined the experiment equipment and its operation. A gas-law analysis was made that included all of the potential contributors to pressure variation. The temperature distributions within the test containers (and, in particular, in the headspace), and temperature variations within the ZPPR cell and within the glovebox were considered. Thermal expansions and contractions of the test vessels, the brine, and the waste materials were evaluated. The vapor pressure (volatility) of the brine constituents, the solubility of the headspace gases in the brine and the accompanying variation in headspace-gas mass, and the compressibility of the brine and the waste were all examined. Corrections to account for changes and errors introduced during calibration of the temperature and pressure transducers were also developed and included, and the reductions in the headspace-gas mass from sample extractions were rigorously included.

Most of these phenomena could be analytically included using parameters available in the literature. A separate experimental apparatus was assembled and used to measure the thermal-expansion characteristics of the liquid brine. Using these parameters, the full analytic treatment was then applied to specific data collected from the experiment-control containers (those that contained brine and microbes, but no waste) to test the methodology. The measured pressure histories for these waste-free containers were as erratic as any, but the pressures that should prevail in the absence of variations in the temperature and other influences, should, of course, be constant.

The full analysis was found to very accurately predict the effects of temperature variation on the pressure. This success with several data points clearly established the general validity of the data. ***The major shortcoming in the earlier analyses was traced to the constant headspace volume assumption, i.e., the omission of the effects of thermal expansion/contraction in the brine and waste.*** This was an unexpected and insidious phenomenon: the small temperature variations that occurred, generally just a few degrees Celsius, affect the volume of the brine/waste only very little. But volumetric changes in the brine/waste are directly impressed on the headspace volume. An increase or decrease in the brine and waste volume causes an equal decrease or increase, respectively, in the headspace-gas volume. Since the brine/waste matrix volume is much greater than the headspace volume, the *relative* volumetric variation in the headspace is amplified by more than an order of magnitude, as compared to that which occurs in the brine/waste. In fact, the brine/waste expansion/contraction phenomenon was found to be the *predominant* effect on test-container pressure, exceeding even the direct effect from variation of the headspace-gas temperature, itself.

1.4.2 Recovery of the Archived Pressure Data

Once it had been demonstrated that the causes of the pressure behavior were fully explainable and quantifiable, a method to nullify these effects in the several years of archived data for the waste-bearing containers was investigated. A key parameter to the methodology was the unknown sensitivity of the brine/waste volume to temperature changes. The method pursued involved deliberately introducing temperature steps in each test container and measuring the corresponding pressure response. This technique allowed the indirect determination of the thermal expansion-contraction characteristics of the brine and waste materials together, a parameter not otherwise known. This obviated the need to physically duplicate the brine/waste and measure the thermal-expansion characteristics in a separate experiment, as had been done for the brine alone, described in the previous section.

With the thermal-expansion characteristics for each waste container known, the full analytic methodology was programmed for computer application and then applied to all of the archived data for each test container. This produced a derived set of pressure-trend data from which the effects of variations in temperature, headspace-gas-mass variation from gas sampling and gas solubility variation, and instrument-calibration errors had been purged. These “adjusted” pressure trends made it possible to deduce the gas-generation rates.

1.5 Organization of the Report

This report describes the analytic investigation of the erratic pressure variation observed. Section 2.0 describes the GGE experiments, the hardware being used, and the general operation. Section 3.0 presents an overview of the data that had been collected. The analysis methodology is outlined in Section 4.0. Section 5.0 discusses the variability of the headspace-gas mass, and Section 6.0 discusses the headspace volume. The thermodynamic parameters for compressibility and temperature are developed in Section 7.0. Temperature distributions are discussed in Section 8.0. These effects are consolidated and a demonstration of the validity of the GGE data is presented in Section 9.0. Section 10.0 describes how the archived data was reconstructed, and Section 11.0 discusses the results and interprets these for evidence of gas generation. Section 12.0 discusses the applicability of the analytic adjustment of pressures to other

experiment programs. Finally, a discussion of the limitations of the analysis is provided in Section 13.0. Back-up materials are provided in several appendices.

The work reported here was largely developed in the latter half of 1998 through Spring 1999, i.e., covering about the first 3.25 years of GGE operation. The calculation was then programmed for computation on a desktop computer. The methodology was outlined and the results were reported to the sponsor as they were developed. This served to resolve the question of data validity and provided the basis for continuation of the program. Complete documentation of the work by this report, along with minor refinements to the analyses, were conducted on and off at a relatively low-priority level from that time through 2002.

2.0 GGE Experiment Configuration

2.1 Test Container Description

Figure 3 was extracted from ANL Drawing No. W0421-0125-ED, Sheet 1 and shows a vertical cross section of the test containers. The test containers were designed for a maximum safe working pressure of 19.995 MPa gage (2900 psig) at 30°C. To minimize gas generation from corrosion of the test containers themselves (gas generation only from interactions among the brine and waste materials are the object of the tests) the bodies, top head, and all miscellaneous parts and fittings within the containers were fabricated from Hastelloy-C276 (Unified Material Number System (UNS) N10276). The diametrically split clamping ring, which has no contact with the brine/waste, was made from American Iron and Steel Institute (AISI) 4140 (UNS G41400) chromium-molybdenum steel. All penetrations into the vessel were through the top head. The numerous penetrations served several purposes: brine addition, sparging, headspace gas access, two thermowells for temperature-sensing instruments (resistance temperature detector [RTD]), and a fitting to connect to a rupture disk assembly for over-pressure protection. Twenty compression bolts clamp the head to the vessel body. A diamond-cross-section, Hastelloy-C276 metal gasket seals the head to the body. A perforated Hastelloy-C276 plate mounted on 50-mm-long standoffs hangs from the bottom of the vessel head to ensure that the waste materials remained fully submerged in the brine and cannot float into the headspace volume.

Wastes were loaded into the test containers in a separate area. The containers were transferred into the argon-filled GGE glovebox (described in the next section) where the inoculated brine was carefully added. The lids were fastened to the containers, and the containers were then purged for approximately 24 h with a 99% nitrogen (N_2), 1% helium (He) mixture injected through the sparging manifold at the bottom of the container to displace the argon. Following the purge, the containers were pressurized with the N_2/He mixture to 17.237 MPa (2500 psia) and checked for leakage using commercial helium leak-detection equipment. After passing the leak check, the pressure was reduced to the WIPP lithostatic pressure of 14.824 MPa (2150 psia), and the test period commenced.

2.2 Glovebox

The test containers were placed inside a large, controlled-atmosphere glovebox. Each test container's clamp ring rests on the upper end of a vertical, double-walled, cylindrical shroud that surrounds the test container. This arrangement keeps the underside of each test container approximately 15 mm (0.6 in.) above the floor of the glovebox. Three electric heater belts were mounted within the annulus of the double-walled shroud and wrapped tightly around the inner wall.

Figure 4 shows the heater configuration prior to installation of the outer wall of the concentric shroud. One heater belt provides ample power; the two additional belts were installed spares. The lowest belt was used initially for all test containers, and no failures were experienced.

Fig. 4. Test-Container Shroud and Heater-Band Arrangement

When fully assembled, the test containers were as depicted in Fig. 5. The pressure is measured by an extremely accurate and stable pressure transducer mounted on a 3-mm-ID standoff tube above the container. The entire instrumentation connections are shown in Fig. 6.

The glovebox is shown in Fig. 7, extracted from ANL-West Drawing No. W0421-0030-ED. The test containers were surrounded by a false floor that had loose-fitting holes through which each test container assembly was placed. When in place, approximately the upper one-third of the test containers protruded above the false floor. Gas blowers circulated purified argon gas through the

glovebox. The gas was circulated through two activated beds, alternately regenerated, to remove oxygen and other impurities. The temperature within the glovebox was measured by an RTD that resided in a pocket located underneath the false floor as shown in Fig. 7.

Fig. 5. Assembled Test Container

3.0 Overview of the Measured Data

Examination of the data from a typical GGE test container is helpful in understanding the problem that was addressed. The temperature measured by the test-container RTD located in the thermowell shown in Fig. 3 is shown in Fig. 8. The deliberate increase in the test container temperature to about 39.8°C, as was alluded to in Section 1.3 and Fig. 1 and Fig. 2, can be seen in Fig. 8 at about Data Point No. 16000. Figure 8 also shows the trace of the temperature measured by the glovebox RTD (see Fig. 7 for the glovebox RTD location). The ZPPR cell air conditioning was turned off at the beginning of the GGE tests, and the rise in the facility and glovebox temperatures are evident. After about 16 months and an unexpectedly hot summer, the facility air conditioning was turned back on (Point No. 2), and its effect in rapidly lowering the ZPPR cell temperature and the glovebox temperature is clearly evident. Prior to the activation of the cell air conditioning, the temperature of the glovebox and test container are clearly synchronized, time wise. Furthermore, it is evident that between Points No. 1 and No. 2 the glovebox temperature had risen so high that the test-container temperature was merely following that of the glovebox, i.e., the test-container's heater controller was no longer active. Following the activation of the ZPPR cell air conditioning at Point No. 2, the lowered glovebox temperature allowed the heaters to regain control of the test-container temperature. Several other activations/deactivations of the ZPPR cell air conditioning are also shown on Fig. 8. Data from this one test container is characteristic of all fourteen GGE test containers.

Fig. 8. Test Container and Glovebox Temperatures for a Typical Test Container (TC-153)

Figure 9 shows the temperature trace from this test container's RTD superimposed on a common abscissa with the pressure trace from the same test container. It can be seen from this plot, as well as in Fig. 1 and Fig. 2, that there is certainly a qualitative relationship between the pressure and

the temperature. Determination of the *quantitative* relationship and the cancellation of any temperature and headspace-gas-mass effects were the objectives of the analysis methodology described in the next several sections of this report.

Fig. 9. Synchronization of Test Container Pressure with Temperature (TC-153)

4.0 Analysis Development

4.1 Application of the State Equation

The GGE test containers were backfilled with nitrogen. A small quantity of helium was added for use as a tracer during leak testing. At normal atmospheric pressure, these gases behave very nearly like thermally perfect gases. However, at increasingly higher pressures, a small deviation occurs. This can be accounted for by the inclusion of a correction, or “*compressibility*”, factor, z , so that an equation of state can be expressed in a form similar to that of a perfect gas as

$$PV_{HS} = zMRT = zNR_U T \quad (2)$$

P is the pressure, V_{HS} is the headspace volume, M is the headspace-gas mass, and T is the absolute temperature. The second form of the equation states the quantity of headspace gas in “moles”, N , where the number of moles is the mass divided by the molecular mass (or molecular “weight” [MW]):

$$N = \frac{M}{[MW]} \quad (3)$$

Expressing the state equation in moles is more useful, since the corresponding gas-constant, R_U , is independent of the particular gas species. The mass-specific gas constants for the generated

gases are markedly different from that for the N_2 bulk fill gas. The predominant generated gas expected is hydrogen. Hydrogen is generated from metal corrosion as well as from the radiolysis of organic waste matter and water. Other potentially generated gases, such as CO_2 and H_2S from microbial metabolism, ultimately attack the abundant carbon steel or aluminum wastes, so they too eventually cause the formation of H_2 . Since the molecular weight of H_2 is so low, approximating its mass-specific gas constant by that for N_2 would not be acceptable, requiring the use of an averaged value, continually changing as the gas composition changed. Although the headspace gas will be quantified in moles and written as N throughout this report, the familiar term “mass” is used when referring to the quantity of headspace-gas matter.

The state equation allows any one parameter to be determined when the others are known. Another way to invoke the state equation is to write Eqn. (2) for one set of conditions and divide that equation by the same equation written for a second set of conditions. This allows, for example, the pressure to be expressed in terms of a known pressure. Given a set of arbitrarily selected reference conditions for which the parameter values are known, denoted by a zero subscript, the pressure at another set of conditions (those without subscripts) is

$$P = P_0 \left(\frac{z}{z_0} \right) \left(\frac{N}{N_0} \right) \left(\frac{V_0}{V} \right) \left(\frac{T}{T_0} \right) \quad (4)$$

Evaluation of the right-hand side of Eqn. (4) will predict the pressure at any point when the reference pressure, P_0 , and the ratios of the four other thermodynamic parameters have been accurately specified. In particular, for each GGE test container, a point-by-point evaluation of Eqn. (4) with the corresponding parameter ratios will predict the actual pressure history relative to some reference pressure. The pressure behavior determined this way can be compared to the pressure history recorded by the data-acquisition system. A suitable match validates the data; a mis-match would indicate that either the data is invalid, the theory is incorrect or incomplete, or that the parameters have not been properly specified.

An equivalent way to apply the methodology is to rearrange Eqn. (4) to give the reference pressure in terms of the measured pressure as

$$P_0 = P \left(\frac{z_0}{z} \right) \left(\frac{N_0}{N} \right) \left(\frac{V}{V_0} \right) \left(\frac{T_0}{T} \right) \quad (5)$$

With this formulation, when the measured pressure at any data point, P , and the other parameters are substituted into Eqn. (5) the selected reference pressure, P_0 , should be found. The error between the calculated estimate and the actual (constant) reference pressure is an indicator of the accuracy of the methodology. This is the form used in this report and will be developed further in subsequent sections.

4.2 Analysis Approach

Each of the terms in Eqn. (4) or (5) refers to properties of the headspace gas, and subsequent reference to these terms in this report have a *g* (gas) subscript appended to these terms to differentiate these from the corresponding parameters in the brine/waste wherever ambiguity may otherwise result (e.g., temperature). The value of each of these terms at any point in time depends on the transient response of the test containers to variations in their surroundings, such as temperature changes in the ZPPR cell, in the glovebox, or heater activation. When any such change occurs, the test containers will begin to respond, gradually adjusting to whatever the new conditions and the physics of the system dictate. However, since the time frames of these external variations are rather long, on the order of several hours, the lag between these external “forcing functions” and the test container response should be small. For this reason, all parts of the test containers are presumed to be in constant and complete thermal equilibrium with their surroundings at all time. This assumption permits the response of the headspace gas to be analyzed as a succession of steady states, instead of calculating the actual transient response. That is, for a set of external forcing functions, the parameters in the headspace gas are presumed to be fixed and can be calculated as if the external conditions at any given instant had prevailed indefinitely. *The genesis of the new state is simply discarded.* Consistent with this approach, only the comparison of the external conditions to those at some arbitrarily chosen, fixed “reference” time need be known to determine the current state. This is an important characteristic of the present analysis. It will be shown, however, that this simplification does not impose serious limitations for the current application.

Having greatly simplified the problem by adopting a quasi-steady approach, **the resolution of the GGE pressure behavior is reduced to an evaluation of Eqn. (5) for each data point for each of the test containers.** The process is straightforward and ostensibly quite simple, but requires meticulous attention to the physics to properly account for all of the important phenomena that are occurring. The challenge in performing the analysis stems from the fact that, aside from the pressure, none of the parameters in Eqn. (5) was directly measured. Each ratio must be deduced from the only measurements that were made: the headspace total pressure and the brine/waste and glovebox temperatures. Accordingly, the majority of this report concerns the development of suitable expressions for the mass of headspace gas, N , the headspace volume, V_{HS} , the headspace-gas compressibility, z , and the headspace-gas temperature, T_g . Several appendices provide supporting materials.

5.0 Headspace-Gas-Mass Considerations

The quantity of gas within the headspace plays a significant role in the analyses. Expressions for this parameter are developed in this section.

5.1 Headspace-Gas Composition and Volatility

The headspace in each test container was backfilled with gas having a volumetric composition of approximately 99% nitrogen and 1% helium. Traces of other gases, principally argon, remained from handling the open test containers and gas-sampling operation in the argon-filled glovebox despite extensive purging with the nitrogen/helium fill gas after the containers were sealed. Equations (4) and (5) are applicable to each of the gas species present in the headspace when z

and N refer only to that particular specie, and P is the partial pressure of that specie. The measured pressure is the sum of all partial pressures. Inclusion of the actual initial gas composition is straightforward, but yields results that are virtually indistinguishable from those found by approximating all of the headspace gas simply as nitrogen. Since the additional calculational complexity from treating gas species separately serves no useful purpose, the headspace gas was subsequently approximated as 100% nitrogen, and properties and parameters for the headspace gas are those for nitrogen in the remainder of this report.

In addition to gas species, there will be some vapor present in the headspace from the vaporization/condensation of the brine. The full pressure is the sum of the partial pressures of all of the gases, both condensable and non-condensable (non-condensable refers to the behavior at room-like temperatures). The subscript g refers to the gas (approximated here as pure nitrogen), and the subscript v refers to the condensable vapor, i.e.,

$$P = P_g + P_v \quad (6)$$

For modest rates of temperature change the headspace will continually be saturated with vapor at the partial pressure corresponding to the local vapor pressure. Water vapor is the only appreciable condensing species at room-like temperatures, so the partial pressure of the vapor, P_v , can be found immediately for a given temperature from saturation data for water, viz., the “steam tables” [1]. Since the partial pressure of the gas specie is equal to the measured pressure minus the partial pressure of the vapor, Eqn. (4) can be applied directly to the non-condensing gas species (nitrogen), as

$$P_g = P - P_v = (P - P_v)_0 \left(\frac{z}{z_0} \right) \left(\frac{N}{N_0} \right) \left(\frac{V_{HS_0}}{V_{HS}} \right) \left(\frac{T_g}{T_{g_0}} \right) \quad (7)$$

The volume in Eqn. (7) is the total headspace volume, and the gas and vapor in the headspace are assumed to be in equilibrium at a common temperature. Similarly, Eqn. (5) can be written

$$P_0 - P_{v_0} = (P - P_v) \left(\frac{z_0}{z} \right) \left(\frac{N_0}{N} \right) \left(\frac{V_{HS}}{V_{HS_0}} \right) \left(\frac{T_{g_0}}{T_g} \right) \quad (8)$$

The actual headspace gas mass at any point in time probably differs from that at the reference point. The totality of the *increase* in the headspace-gas mass relative to the mass at the reference point is written as ΔN . Therefore, the headspace-gas mass at any specific point being analyzed is

$$\begin{aligned} N &= N_0 + (N - N_0) \\ &= N_0 + \Delta N \end{aligned} \quad (9)$$

The mass ratio in Eqn. (8) can then be written as

$$\frac{N_0}{N} = \frac{N_0}{N_0 + \Delta N} \quad (10)$$

Once ΔN has been determined, this ratio can be calculated. The remainder of this section considers the various phenomena that produce variation, ΔN , in the headspace-gas mass.

5.2 Sources of Variation in the Headspace-Gas Mass

The mass of gas within the headspace can vary for several reasons. There are two types of variation that the test containers are subjected to that are *discrete*, i.e., occurring only at specific times: (1) at each headspace-gas-sampling a small quantity of gas is physically extracted from the headspace for analysis; and (2) because of the particular technique required, the periodic calibration of the pressure transducer (PXD) introduces a potential for inadvertently altering slightly (either increasing or decreasing) the headspace-gas mass. A less obvious mass change may occur at any time as a result of variation in the quantity of headspace gases dissolved in the brine. Solubility of a given gas in the brine depends on the pressure of the gas species in the headspace and the brine temperature. Solubility variation acts like a source or sink of gas to the headspace. Finally, of course, there may have been gases generated within the brine as a result of microbial metabolism, radiolysis, or corrosion. Solubility variation and gas generation are continuous changes, or at least piece-wise continuous over short segments of time.

The total change in headspace mass can be resolved into its contributors, per the above discussion:

$$\Delta N = \Delta N_{sampling} + \Delta N_{pxd} + \Delta N_{sol} + \Delta N_{gen} \quad (11)$$

Each of these terms represents the total increase (algebraically summed) with time in the headspace-gas mass as a result of sample extractions, PXD calibrations, solubility variation, and gas generation, respectively, between the current point and the reference point. With this expression, Eqn. (8) becomes

$$P_0 - P_{v_0} = (P - P_v) \left(\frac{z_0}{z} \right) \left(\frac{N_0}{N_0 + \Delta N_{sampling} + \Delta N_{pxd} + \Delta N_{sol} + \Delta N_{gen}} \right) \left(\frac{V_{HS}}{V_{HS_0}} \right) \left(\frac{T_{g_0}}{T_g} \right) \quad (12)$$

Each of the contributors to the mass increase, except for the gas-generation, can be evaluated from conditions measured in the experiment. Expressions for the difference (increase) in headspace gas mass between a given point and the reference point for each of the non-gas-generation components are developed in the following sections.

5.2.1 Discrete Headspace-Gas-Mass Variation

The two discrete-change components of ΔN , i.e., from gas sampling and the PXD calibrations, can be written, for brevity, as a single term, ΔN_D , where by definition,

$$\Delta N_D = \Delta N_{sampling} + \Delta N_{PXD} \quad (13)$$

Gas sampling and PXD calibrations occur only at specific discrete points, where a discrete change of magnitude δN_{D-i} is experienced. This term is algebraic: always negative for a sampling

event, and either positive or negative for a PXD-calibration event. Consider the relationship between ΔN and δN for some hypothetical sequence of headspace-gas-mass changes that result from any discrete phenomenon. For example, between Point-A and the reference point in Fig. 10 there are two mass additions (events 1 and 2) and two mass extractions (events 3 and 4), having arbitrary magnitude. Similar headspace-gas-mass-change events occur at points beyond the reference point to some Point-B. Starting from Point-A, it is easily seen that

$$N_A + \delta N_4 + \delta N_3 + \delta N_2 + \delta N_1 = N_0 \quad (14)$$

Fig. 10. Representation of Discrete Events at Times Prior To and Beyond the Reference Point

The quantities δN_4 and δN_3 are decreases (negative); δN_2 and δN_1 are increases (positive). Comparing Eqn. (14) to Eqn. (9), at points *prior* in time to the reference point, the difference between headspace-gas mass at a given point and that at the reference point is

$$\Delta N = N_A - N_0 = - \sum \delta N_i \quad (15)$$

Similarly, *beyond* the reference point to Point-B an analogous development shows

$$N_0 + \delta N_1 + \delta N_2 + \delta N_3 + \delta N_4 = N_B \quad (16)$$

In this case,

$$\Delta N = N_B - N_0 = + \sum \delta N_i \quad (17)$$

Generalizing this to the case where there are a total of J *discrete* events that occur between some point and the reference point,

$$\Delta N_D = \mp \sum_{i=1}^J \delta N_{D_i} \quad (18)$$

For points prior in time to the reference point the negative sign is to be used; the positive sign applies to points beyond the reference point.

The discrete events occur nearly isothermally, and typically involve only very small pressure changes, on the order of 55-69 kPa (8-10 psi), a variation of less than 0.5% of the 14.824-MPa (2150-psia pressure). The variation in compressibility is even smaller (on the order of 0.03%). The mass change over the i^{th} such discrete event can therefore be found by expressing the mass terms with the equation of state, Eqn. (2), and differentiating, giving

$$\delta N_{D_i} = \frac{V_{HS} \delta P_{g_i}}{z R_U T_g} - \frac{P_g V_{HS} \delta z}{z^2 R_U T_g} \approx \frac{V_{HS} \delta P_{g_i}}{z R_U T_g} \quad (19)$$

Pressures and temperatures were recorded during the discrete events. Use of these pressures in Eqn. (19) allows the determination of the mass change at each discrete event once V_{HS} is known. The headspace volume that pertains to each discrete event for use in Eqn. (19) is discussed in Section 6.0.

5.2.2 Continuous Headspace-Gas-Mass Variation

Variation in the headspace-gas mass as a result of continuous (subscript C), or piece-wise continuous, changes are not intrinsically different than discrete changes. In the most general case, over some specific time interval, δt_i , a change in the headspace-gas mass occurs of magnitude δN_{C-i} , where

$$\delta N_{C_i} = \int_{\delta t_i} dN_C = \int_{\delta t_i} \frac{dN_C}{dt} dt = \int_{\delta t_i} \dot{N} dt \quad (20)$$

If there are K intervals over which continuous changes occur, then by analogy to the preceding section

$$\Delta N_C = \mp \sum_{i=1}^K \delta N_{C_i} \quad (21)$$

As was the case for the discrete variation, the negative sign is used for intervals prior to the reference point and the positive sign is used beyond the reference point.

The values of J and K in Eqn. (18) and Eqn. (21) refer only to the number of headspace-gas mass-change events that actually fall between the calculational point being considered and the reference point. Therefore, the values for each of J and K are unique to each point, and those values at one calculational point will likely differ from those at other points.

5.2.3 Gas-Solubility Variation

By definition, at any gas pressure the mole fraction of a dissolved gas (subscript *dis*) in a liquid (subscript *l*) is

$$x = \frac{N_{dis}}{N_l + N_{dis}} \quad (22)$$

The *increase* in headspace-gas mass equals the *decrease*, i.e., the negative of the increase, in the mass of the dissolved gas. Thus, the solubility-variation contribution to the overall gas-mass variation in the headspace is given by the negative of the difference between the dissolved gas mass at the current calculational point and the dissolved-gas mass at the reference point. Using this,

$$\Delta N_{sol} = - \Delta N_{dis} = - (N_{dis} - N_{dis_0}) = N_{dis_0} - N_{dis} \quad (23)$$

The dissolved gas quantity can be computed from Eqn. (22), so that

$$\Delta N_{sol} = N_l \left(\frac{x_0}{1 - x_0} - \frac{x}{1 - x} \right) \quad (24)$$

The *equilibrium* quantity of gas dissolved can be determined using solubility relationships found in the literature. For a given gas/solvent combination, Reference 3 gives the mole fraction of gas dissolved in the brine, X_{dis} , when the partial pressure of that gas above the liquid surface is one atmosphere as

$$\log_e X_{dis} = A + \frac{B}{T'} + C \log_e T' \quad (25)$$

The term T' is a non-dimensional temperature defined by $T' = T/100$ K, and A , B , and C are gas/solvent-specific constants. For nitrogen gas in *water*, the constants A , B , and C are -67.3877, 86.3213, and 24.7981, respectively (3). Nitrogen is the predominant gas in the headspace. Although there are much more soluble gases that may be present as a result of gas generation, e.g., CO_2 or H_2S , these would be expected to be present in such limited quantities that even

significant variation in their solubilities would have only a minor effect on the total headspace-gas mass. These values were presumed to pertain to solutions of nitrogen in *brine*, as well. The mole fraction of gas dissolved at the actual conditions is very nearly proportional to the actual partial pressure of the gas (Henry's Law). Therefore, the mole fraction of gas dissolved at the prevailing pressure is

$$x = X_{dis} P_g \quad \text{where } [P_g] = atm \quad (26)$$

Reference 7 cites some slight variation in this proportionality, but the variation is sufficiently small to ignore here. Equations (25) and (26) can be substituted into Eqn. (24) to calculate the variation in the mass of gas dissolved in the brine at the actual pressure.

The solubility relations presented above refer to equilibrium conditions. Like the transient thermal response discussed in Section 4.2, an accurate determination of the quantity of gas dissolved in the brine at any time requires a consideration of the mass-transfer dynamics. The present quasi-steady analysis cannot account for transient effects: a choice must be made to either omit the solubility effects altogether (appropriate for very sluggish mass-transfer dynamics) or include the solubility at the equilibrium values (appropriate for very rapidly equilibrating dynamics).

Mass-transfer dynamics are examined in Appendix A. It is demonstrated there that changes in the quantity of gas dissolved in a quiescent liquid occur very slowly for nitrogen, because of its low mass-diffusion coefficient. Furthermore, the measured variations in temperature and pressure during the GGE program tended to be erratic (non-uniform, certainly, but roughly alternately increasing and decreasing relatively rapidly). Such oscillations tend to limit the penetration of any transported quantity. This effect is similar to the approximately constant soil temperature that persists just a few millimeters below the earth's surface despite significant diurnal variation in the surface temperature. As it turns out, inclusion of the solubility contributions in the calculation program even at the equilibrium values yields results that are virtually indistinguishable from those for which solubility effects were omitted, indicating that the effect is second order, at best, insofar as compensation for the variable external effects are concerned. Solubility effects may be significant if there were ample quantities of other, very soluble, gases, such as CO_2 or H_2S , and the long-term effects of solubility on the WIPP depository performance may well be important. These issues were not considered in the present work.

Although unimportant for this situation, the solubility term is included in the remaining development in this report for completeness.

5.3 Gas-Generation-Rate Specification

5.3.1 Increase in Headspace-Gas Mass by Gas Generation

The gas-generation term in Eqn. (12) can be solved for explicitly to give

$$\Delta N_{gen} = \frac{P - P_v}{P_0 - P_{v_0}} \left(\frac{z_0}{z} \right) N_0 \left(\frac{V_{HS}}{V_{HS_0}} \right) \left(\frac{T_{g_0}}{T_g} \right) - (N_0 + \Delta N_D + \Delta N_{sol}) \quad (27)$$

This equation then gives the quantity of gas generated between the present calculation point and the reference point once the thermodynamic parameters have been specified. However, the first objective of this work was to demonstrate the validity of the data by examining the “blank”, experiment-control test containers (Test Containers No. 152 and 153) for which there could be no gas generation. To do this an alternate form for gas generation is more useful, as developed below.

For the blank test containers, it would be expected that the pressure would be constant after the effects of temperature and headspace-gas-mass variation have been properly nullified. Examination of the two non-waste-bearing containers also serves to find out if the measured pressure, with all of its observed variation, could have been adequately predicted by the present analytical methodology. For this reason, Eqn. (12) is re-written ignoring gas generation, i.e., variations in the headspace-gas mass are assumed to result only from non-gas-generation phenomena. The *pressure computed with the specific presumption of no gas generation* is designated as simply the “adjusted” pressure, i.e.,

$$P_{adj} - P_{v_0} = (P - P_v) \left(\frac{z_0}{z} \right) \left(\frac{N_0}{N_0 + \Delta N_D + \Delta N_{sol}} \right) \left(\frac{V_{HS}}{V_{HS_0}} \right) \left(\frac{T_{g_0}}{T_g} \right) \quad (28)$$

A match of the adjusted pressure at all points to the reference pressure validates the data by demonstrating that the seemingly erratic variation in the measured pressure was, in fact, the expected thermodynamic consequences of temperature and headspace-gas-mass variation. This can be seen clearly by comparing equations (12) and (28).

An adjusted pressure per Eqn. (28) can be computed for all of the test containers, of course, including those bearing potentially gas-generating waste. The motive is that since the adjusted pressure accounts for all of the thermodynamic phenomena that are occurring *except* gas generation, any non-constant behavior would identify the occurrence of gas generation. Having chosen to compute P_{adj} , as defined by Eqn. (28), it can be used to specify the mass of gases generated as an alternate to Eqn. (27). Dividing Eqn. (28) by Eqn. (12) eliminates the thermodynamic terms, including the measured pressure at the given point, giving

$$\frac{P_{adj} - P_{v_0}}{P_0 - P_{v_0}} = \frac{N_0 + \Delta N_D + \Delta N_{sol} + \Delta N_{gen}}{N_0 + \Delta N_D + \Delta N_{sol}} \quad (29)$$

This can be rearranged to give the quantity of gas generated explicitly as

$$\Delta N_{gen} = \frac{P_{adj} - P_0}{P_0 - P_{v_0}} (N_0 + \Delta N_D + \Delta N_{sol}) \quad (30)$$

Before concluding the discussion of headspace-gas mass, two other useful representations of the generated-gas mass are developed in the following two sections.

5.3.2 Mole Fraction of Generated Gases

Measurements of headspace-gas composition for low concentrations are usually reported as volume fractions of each specie, e.g., as parts per million by volume, ppm/V. The mole fraction is equivalent to a volume fraction for an ideal gas. In the present case, the increase in the mole fraction of the generated gas, ΔX_{gen} , at any time relative to that value at the reference point is

$$\Delta X_{gen} = \frac{\Delta N_{gen}}{N} = \frac{\Delta N_{gen}}{N_0 + \Delta N_D + \Delta N_{sol} + \Delta N_{gen}} \quad (31)$$

Substituting Eqn. (29) into this equation gives

$$\Delta X_{gen} = \frac{P_{adj} - P_0}{P_{adj} - P_{v_0}} \quad (32)$$

Equation (32) shows the usefulness of P_{adj} in identifying and quantifying gas generation, i.e., $P_{adj} - P_0$ non-zero indicates gas generation.

The increased mole fraction of gas generated between any two points, e.g., Point *a* and Point *b*, is equal to the mole fraction increase at a Point *b* vis-a-vis the reference value minus the mole-fraction increase at Point *a* relative to the same reference value, as demonstrated below:

$$\begin{aligned} \delta X_{gen} &= X_{gen-b} - X_{gen-a} = X_{gen-b} - X_{gen-0} + X_{gen-0} - X_{gen-a} \\ &= \Delta X_{gen-b} + (-\Delta X_{gen-a}) \\ &= \Delta X_{gen-b} - \Delta X_{gen-a} \end{aligned} \quad (33)$$

The term δX_{gen} would be positive for positive gas generation, and negative for negative gas-generation. Although negative gas generation, as such, is purely hypothetical, it would be analogous to absorption or dissolution of gas into the brine.

5.3.3 Rates of Gas Generation

The *rate* of gas generation is also typically of interest. This is simply the slope of the gas-generation rate, and can be readily inferred from a plot of ΔX_{gen} , per Eqn. (33). The gas-generation rate should be calculated as an average over a sufficiently large time interval, δt , so that point-to-point variation in the gas-generation data is adequately filtered. This time interval can be related to time intervals with respect to the reference point by a development analogous to that for Eqn. (33), giving

$$\delta t = \Delta t_b - \Delta t_a \quad (34)$$

The average rate of change of the mole fraction of generated gas in the headspace over the time interval is, therefore,

$$\dot{X}_{gen} = \frac{\delta X_{gen}}{\delta t} = \frac{\Delta X_{gen_b} - \Delta X_{gen_a}}{\Delta t_b - \Delta t_a} \quad (35)$$

This can be evaluated from Eqn. (32).

6.0 Headspace Volume Considerations

The volume of the test container headspace, V_{HS} , will be shown to play a very important role in the solution. Its value is not as obvious as it may first appear, as demonstrated in the development in this section.

6.1 Headspace Volume Variation

Consistent with the deviation-from-a-reference-point approach being used in this analysis, the headspace volume at some given condition is related to the headspace volume at the reference conditions (zero subscript) by

$$V_{HS} = V_{HS_0} + \Delta V_{HS} \quad (36)$$

The headspace volume is the volume remaining in the container (subscript c) after the volume occupied by the brine/waste (“liquid”, subscript l) has been subtracted:

$$V_{HS} = V_C - V_l \quad (37)$$

Differentiating Eqn. (37) and expressing the differential over a small but finite interval gives the increase in headspace volume as directly related to the increases in volumes of the test container and the brine/waste:

$$\delta V_{HS} = \delta V_C - \delta V_l \quad (38)$$

The test container undergoes expansion and contraction as the temperature and pressure change, as do the volumes of brine and each waste constituent. These effects are impressed on the headspace-gas volume, and act in opposite directions. For example, when the temperature rises the test container expands and the internal volume increases slightly, acting to increase the headspace volume. But the simultaneous thermal expansion of the brine/waste acts to decrease the headspace volume. Development of these two competing effects are presented in the following two sections. These seemingly minute effects, induced by very small temperature and pressure changes, will be found to have the most significant consequences for the pressure behavior.

6.1.1 Test-Container Expansion/Contraction

At conditions different from those at the reference conditions the test-container volume is

$$V_C = V_{C_0} + \Delta V_C \quad (39)$$

The test container volume depends on its temperature and the differential pressure loading across its boundaries. The latter effect results from variation in the vessel strain caused by changes in the internal pressure relative to the nearly constant glovebox pressure. However, given the extreme stoutness and strength of the containers, the vessel-strain variations can be quickly shown to be fully negligible. Therefore, only the expansion/contraction from thermal effects needs to be considered.

Let the container internal free volume at some known temperature be V_C , and let α denote the coefficient of *linear* thermal expansion of the material of construction. The volume of a container of any shape is proportional to a linear dimension cubed. Invoking this relationship, it can be easily shown that, regardless of the geometric shape of the container, a uniform, infinitesimal temperature change of amount dT from the given state causes a corresponding volume change, dV_C , of amount

$$dV_C = 3\alpha V_C dT \quad (40)$$

This form can be used directly for small temperature changes, δT , to give δV_C . Since α , itself, frequently is temperature dependent, the average value of α over the given temperature interval is taken for larger temperature changes. Upon integrating Eqn. (40), the test-container volume increase is found to be

$$\delta V_C = V_{C_0} (e^{3\bar{\alpha} \delta T_{RTD}} - 1) \quad (41)$$

If necessary, this expression can be adapted to the case where the temperature change over the container boundaries is non-uniform by integrating Eqn. (41) over the entire vessel. However, as is discussed later concerning the thermal model, the assumption of uniform temperatures in the vessel barrel at the temperature of the RTD immersed in the brine/waste is quite adequate, allowing Eqn. (41), written relative to the reference point, to be used directly in Eqn. (39).

The free volume of the empty test containers was calculated from dimensional data shown on the design drawings. The volume was calculated to be 7272 ml at the nominal temperature that prevailed during manufacture, assumed to be normal room conditions. Any error in determining the vessel's reference volume has only a small effect on the pressure calculation. Since the experiments were carried out at very near room temperature, the reference volume was therefore simply taken to be 7272 ml at whatever particular reference conditions were selected.

6.1.2 Expansion/Contraction in the Brine and Waste

Volumetric changes in the brine/waste result from both temperature and pressure changes, just as was the case for the test container. An argument similar to that made for the vessel strain was made for the brine/waste as well, viz., that pressure effects are negligible—the brine/waste is assumed to be fully incompressible. This, however, may not actually be true. The brine volume can certainly be shown to be negligibly affected by modest pressure changes, but the response of the waste materials themselves, is less certain. Waste materials may include some relatively compliant constituents, such as rubber, that have relatively low moduli of elasticity. Or, worse still, there may be some trapped gas bubbles among the waste, particularly among the debris-types of waste. Since there was no way to accurately assess this, only the *thermally* induced expansion/contraction of the brine/waste was accounted for in the methodology.

Defining a *volumetric* coefficient of thermal expansion for the brine/waste combination as β , the change in volume of the brine/waste due to thermal expansion is, by definition,

$$dV_l = \beta V_l dT_l \quad (42)$$

Similar to the test container thermal expansion, where temperature changes from the reference value are small, this form can be used directly to compute the brine/waste volume change (increase), δV_l . For larger temperature intervals, the change should be computed by integrating Eqn. (42) over the interval and using the average value of β over the interval, resulting in

$$\delta V_l = V_{l_0} (e^{\bar{\beta} \delta T_{RTD}} - 1) \quad (43)$$

The similarity between Equations (41) and (43) is apparent. However, it should be appreciated that the coefficient of *linear* expansion for the container, α , pertained to a unique, solid, engineering material and can be readily found in the literature. In the present case, β refers to the *volumetric* expansion of a composite concoction of brine and waste materials. There are no tabulations for this parameter; its value must be determined experimentally, as is discussed later in Sec. 10.1.

Writing Equations (38), (41), and (43) relative to the reference point and substituting these into Eqn. (36) gives the headspace volume at the current point as

$$V_{HS} = V_{HS_0} + \Delta V_{HS} = V_{C_0} e^{3\bar{\alpha} \Delta T_{RTD}} - V_{l_0} e^{\bar{\beta} \Delta T_{RTD}} \quad (44)$$

6.2 Headspace Volume Determination

The headspace volume at the reference conditions, V_{HS-0} , was not known. This warrants an explanation. The initial brine/waste volume was not measured prior to loading the test containers,

so the headspace volume could not simply be determined by subtracting the brine/waste volume from the container free volume via Eqn. (37). Although the masses of waste and brine added to each container were carefully recorded, the densities of the waste materials were not known exactly, and certainly not when submerged in the brine and at operating conditions. The headspace volume was found by gas-expansion measurements, as described in the next section.

6.2.1 Headspace-Gas Expansion Measurements

The GGE project determined the headspace volume indirectly by carefully measuring the pressure both before and after an expansion of the headspace gas by appending to the headspace a very small, accurately known volume used to extract a headspace-gas sample. Figure 11 depicts the experimental configuration for determining the headspace volume.

Fig. 11. Depiction of the Headspace Volume Measurement

The mass of gas in the headspace after the gas expansion would be affected if there were a change in the amount of gas dissolved in the brine, and this would influence the gas pressure.

Solubility effects can be accounted for by recognizing that the total mass of gas within the test container (i.e., the sum of gas in the headspace plus that dissolved in the brine) is constant during the short time span of the sampling event, during which there would be negligible gas generation. Therefore, the mass of gas within the headspace after the expansion must equal that present prior to the expansion plus the change that occurred only as a result of solubility variation. Letting subscripts 1 and 2, respectively, represent the headspace conditions before and after the expansion of the gas across Valve A (Fig. 11) into the known sample volume, V_s , the final headspace-gas mass is

$$N_2 = N_1 + \delta N_{sol} \quad (45)$$

During the brief time required for the expansion, there are no appreciable gases generated. The gas volume after the expansion is just $V_{HS} + V_s$. Invoking Eqn. (6) with Eqn. (2), as written for the conditions both before and after the expansion, and combining the equations with Eqn. (45) gives the headspace volume deduced from the pressure measurements as

$$V_{HS} = \frac{V_s \frac{P_2 - P_{v_2}}{z_2 T_{g_2}} - R_U \delta N_{sol}}{\frac{P_1 - P_{v_1}}{z_1 T_{g_1}} - \frac{P_2 - P_{v_2}}{z_2 T_{g_2}}} \quad (46)$$

Analogous to Eqn. (24), solubility variation over the expansion would cause an equilibrium headspace-gas-mass change of amount

$$\delta N_{sol} = N_l \left(\frac{x_1}{1 - x_1} - \frac{x_2}{1 - x_2} \right) \quad (47)$$

Equation (47) can be substituted into Eqn. (46). However, as was noted in Section 5.2.3, the slow dynamics of the gas transport into and out of the brine cause the actual mass change over the short time frame during which the sampling operation occurs to be far less than this equilibrium quantity, so the term in Eqn. (46) containing δN_{sol} can be safely omitted.

The quantities P_1 and P_2 in Eqn. (46) are the pressures measured before and after the gas expansion, respectively. P_{v_1} and P_{v_2} and the temperatures T_{g_1} and T_{g_2} must be deduced from the brine and glovebox temperature measurements. Normally, this expansion is done slowly and isothermally, allowing the temperatures to remain constant. The sample volume, V_s , used in the GGE was determined in a similar way by expanding a gas into a calibrated volume, finding a volume of 3.05 ml (8).

6.2.2 Adjustment of the Headspace Volume Measurements

The headspace volume was measured as described in the preceding section each time a headspace-gas sample was drawn. Typically 5 to 8 such sampling events had occurred for each test container before gas sampling was suspended rather early in the experiment program. Each of these sampling measurements provides a calculated value for the headspace volume *at the conditions for which the measurement was made*. Per the development cited earlier, Eqns. (36) through (44), the headspace volume depends on the temperatures of the brine/waste and the test container. So unless these temperatures were identical for all sampling events, the headspace volume measurements will be slightly different. To compare these measurements, the measured volumes need to first be adjusted to common conditions. Consistent with the present development where all measurements are corrected back to a specific reference, the headspace volume measurements were all adjusted to the selected reference conditions.

Any difference in the headspace-gas *mass* between the time when the sampling occurred and the selected reference point (plus possibly some minor difference in the compressibility factor, z , between the two points), will effect the pressure, but not the headspace volume. So, only the ΔV_C and ΔV_l terms need to be considered, and the relation in Eqn. (36) still holds. Eqn. (44) gives the headspace volume at the sampling point in terms of the unknown volume, V_{l-0} . Let V_{HS-j} denote the raw headspace volume determined for the j th sample as calculated from Eqn. (46). The adjustment of that headspace volume to the corresponding volume that would be found at the reference conditions is as follows. From Eqn. (44), replace V_{l-0} by it equivalent,

$$V_{l_0} = V_{C_0} - V_{HS_0} \quad (48)$$

Then substitute V_{HS} as found from Eqn. (44) into

$$V_{HS_{0j}} = V_{HS_j} - \Delta V_{HS_j} \quad (49)$$

This yields

$$V_{HS_{0j}} = \frac{V_{HS_j} + V_{C_0} \left(e^{\bar{\beta} \Delta T_{RTD_j}} - e^{3\bar{\alpha} \Delta T_{RTD_j}} \right)}{e^{\bar{\beta} \Delta T_{RTD_j}}} \quad (50)$$

Equation (50) can be evaluated immediately when the coefficient β is known. For the case of pure brine, a separate experiment was performed to determine the value of β . The experiments are discussed in Appendix B. In the general brine/waste case, however, β is unknown. Its determination is discussed in Section 10.1. It will be shown in Section 10.1 that β , itself, depends on the headspace volume at the reference conditions. Therefore, a simultaneous solution with Eqn. (50) will be found necessary to determine the adjusted headspace volume, V_{HS-0j} , for each measurement.

Ideally, all of the headspace volume measurements should yield precisely the same value *after having been adjusted to common conditions* (such as at the reference point). However, the individual headspace volume calculations are based on field measurements, so some variation among the measurements must be expected, and this variation carries over to the adjusted values. The j subscript on the adjusted headspace volume in Eqn. (50) emphasizes that this result pertains specifically to the j^{th} field measurement. An arithmetic average over all of the n adjusted volume measurements will yield the best estimate of the true mean volume at the reference conditions:

$$V_{HS_0} = \frac{1}{n} \sum_{j=1}^n V_{HS_0_j} \quad (51)$$

The headspace volumes determined from Eqn. (50) are listed in Table 2, along with their corresponding reference-point temperatures. The headspace volume for each test container allows the corresponding brine/waste volume, V_{1-0} , to be found from Eqn. (48). Then V_{HS} can be calculated from Eqn. (44), allowing the ratio V_{HS-0}/V_{HS} to be evaluated.

Table 2. Best Estimate Headspace Volumes at the Reference Conditions

Test Container No.	Reference Temperature (C)	Headspace Volume (ml)
TC-151	31.1	631
TC-152	31.0	733
TC-153	31.0	727
TC-160	31.1	1080
TC-161	31.3	905
TC-161e ^a	31.2	905
TC-162	30.7	910
TC-163	31.0	945
TC-164	30.8	923
TC-165	30.7	807
TC-166	31.1	765
TC-167	31.3	911
TC-168	31.3	912
TC-169	30.2	849
TC-170	31.1	743

a. TC-161e uses empirical calibration constants for TC-161.

7.0 Headspace-Gas Compressibility

For a truly thermally perfect gas, z implicitly has a constant value equal to unity under all conditions. However, for real gases the compressibility factor, itself, is dependent on temperature and pressure; thus, the apparent simplicity of writing a state equation like Eqn. (2) that includes such a factor is misleading. The compressibility factor can take on values greater or less than unity, depending on specific conditions. The usefulness of specifying the state equation in terms of z lies in the fact that for many applications only the initial and end states are needed. For other processes over a small range, it may be acceptable to approximate z as a constant. In both of these cases, the compressibility factor can be read directly from published tables or plots.

Finding the ratio z_0/z is, in principle, straightforward. The factors can be read directly for a given temperature and pressure from charts like that shown in Fig. 12 for nitrogen, the predominant gas in the GGE containers. However, for the small changes in temperature and pressure that occurred in the GGE, the scale of the compressibility plot is much too small to determine the ratio accurately. Furthermore, for analysis usage, it is preferable to have a mathematical representation so that z can be programmed and calculated. This can be done by using one of the many equations of state that have been proposed to describe the behavior of real gases.

Fig. 12. Compressibility Factor for Nitrogen Gas

The Beattie-Bridgeman equation of state has been found to produce results in excellent agreement to experimental measurements for many gases over a wide pressure range, including those of interest to the GGE. This equation of state was selected for this analysis. The relation is

$$P_g = \frac{[R_u T_g (1 - e)(v_g + B) - A]}{v_g^2} \quad (52)$$

where R_U is the universal gas constant and v_g is the mole-specific volume (2). The constants A , B , and e are defined in terms of various constants specific to a given gas and other thermodynamic parameters:

$$\begin{aligned} A &= A_0(1 - a/v_g) \\ B &= B_0(1 - b/v_g) \\ e &= \frac{c}{v_g T_g^3} \end{aligned} \quad (53)$$

These are units-dependent equations, formulated for units of

$$[P_g] = \text{atm}$$

$$[T_g] = \text{K}$$

$$[v_g] = \text{liter/g-mole}$$

In these units the universal gas constant, R_U , is 0.08206 atm-liter/g-mole/K. For nitrogen, the specific constants needed are (2)

$$\begin{aligned} A_0 &= 1.345 \\ a &= 0.02617 \\ B_0 &= 0.05046 \\ b &= -6.910E-03 \\ c &= 42.00E+03 \end{aligned} \quad (54)$$

The Beattie-Bridgeman equation, however, is awkward to use because it is transcendental. An iterative solution for specified pressure and temperature was performed by evaluating the right-hand side of Eqn. (52) with Eqn. (53) and Eqn. (54), using assumed values of the mole-specific volume, v , until a match to the left-hand side was achieved. An algorithm for rapidly performing this trial solution was developed and included in the computer-calculation program discussed later.

By combining the result with the gas law, Eqn.(2), an analytical expression for the compressibility factor becomes

$$z = \frac{(1 - e)(v_g + B) - \frac{A}{R_U T_g}}{v_g} \quad (55)$$

Evaluating Eqn. (55) at the reference conditions and at the conditions of each data point under consideration allows determination of the ratio z/z_0 . Compressibility factors calculated with this equation for nitrogen show very good agreement to the experimental data shown in Fig. 12 up to about 3000 psia, well in excess of the pressure range applicable to the GGE.

8.0 Headspace-Gas Temperatures

The final term needed for the evaluation of the adjusted pressure, Eqn. (28), and the gas generation rate, Eqn. (35), is the ratio of the temperature in the headspace gas at the current point to the headspace-gas temperature at the reference point. This ratio is developed in this section.

8.1 Equilibrium Temperatures

The temperatures in Eqn. (2) refer, of course, to the that of the headspace gas. However, not only is the temperature in the headspace non-uniform, there was no instrumentation in the GGE experiments to measure any headspace temperature. The test-container temperature was measured by an RTD placed in a thermowell immersed in the brine, as shown in Fig. 3. Examination of the vessel geometry and the typical temperature traces for test container and glovebox RTD's shown in Fig. 8 suggest that the temperature in the headspace gas is not necessarily accurately represented by the thermowell-RTD measurement: the top region of the vessel is surrounded by the cooler glovebox environment that will certainly cause the headspace gas to be somewhat cooler than the brine/waste. Thermal conditions within the test container were therefore modeled to better estimate the true headspace-gas temperature from the limited temperature data.

Two steady-state, finite-difference thermal models were developed. The first was a two-dimensional, axi-symmetric model whose node structure is shown in Fig. 13. The model represented the geometry of the actual vessel quite well, requiring only some small adjustments to smear certain features in the top head and miscellaneous fittings such as the brine-filler tube, etc. to an approximate equivalent in rotationally symmetric geometry. When suitable relations for the thermal conductance in the various regions and at the interfaces were applied, the model could be executed with varying electric power at the heating band location until the calculated temperature at the thermowell location matched the actual RTD measurement. A specified heat source was imposed on nodes $(i,k) = (10,3), (10,4),$ and $(10,5)$ in the discretized model shown in Fig. 13, since only the lowest heating band was energized. The heater power was proportioned among these nodes in relation to the fractional coverage by the heater band on each node. The temperature distribution throughout the entire test vessel would then be known, including, in particular, the average temperature in the headspace gas.

Finding the match of the calculated RTD-node temperature to the measured value is simpler than it may appear *if* the heat transfer in the brine and headspace results only from conduction. First, a normalized, non-dimensional temperature is defined with the bottom wall of the test vessel set to temperature unity, and the glovebox environment set to temperature zero. Execution of the thermal model on this basis and with an assumed value for the heater power will yield a corresponding temperature distribution throughout the model. Because of the linearity of the conduction equation, all of the temperatures may be scaled to find the desired values by using a scale factor equal to the ratio of the target RTD node temperature to the temperature calculated at the node. Only when there are temperature-dependent properties and/or inter-node conductances, or non-linear convective heat-transfer correlations will a scaling approach like this be compromised, but even in that case, the scale factor can be used to guide the second guess for the heater input that will usually yield very good results.

Natural convection in the brine picks up heat from the lower end of the test containers (where the heater band is located) and transports the heat to the brine surface. Upon giving up the heat, the brine is somewhat cooled, increasing its density and causing it to sink back to the bottom of the test container to begin another cycle. This phenomenon creates vertical, recirculating cells of fluid movement. The geometric structure of these cells might range from a single core of warm fluid surrounded by a counter-flowing “jacket” of the cooler fluid (or vice versa) to, more probably, multiple, parallel micro cells of warmed and cooled counter-flowing fluids. A full two-dimensional treatment requires that the convection in this region, and within the headspace region, be modeled two dimensionally. This is a difficult calculation to do accurately, and, in any event, a full two-dimensional analysis will be quite time-consuming to run (the archived data examined for each of the 14 test container over the initial 3.25 years of testing consisted of over 26,000 data points, each point of which requires the thermal model to be executed). Some simplification was therefore investigated to ease this computational burden. This simplification is discussed below.

Gross radial temperature variation results only from heat losses from the sides of the test container. Since the body of the test container is surrounded by a thick gap of confined argon gas, which has a relatively low thermal-conductivity coefficient, radial heat losses in that region should be modest. A much simpler, one-dimensional (axial) thermal model was therefore subsequently developed.

The one-dimensional model is depicted in Fig. 14. This is a simple series heat-transfer model, based on the presumption of only second-order temperature variation radially over the body of the test container. Some adjustments, described shortly, were made to account for two-dimensional effects in the upper region. In this model, all heat is transferred from the lower region of the brine/waste to the container head and then out to the glovebox environment through the top of the vessel head. The mathematic representation is quite simple. The heat flow rate, q , is determined from the series resistances, the inverse of the conductances, h , between the hot and cold temperatures. With reference to Fig. 14,

The four conductance parameters (h 's) can be estimated from various correlations in the literature and are functions of material properties, which are possibly temperature dependent. The five unknown quantities are q , T_0 , T_1 , T_2 , and T_3 . The five relations given in Eqn. (56) and (57) are not linearly independent, however, since Eqn. (57) is just the sum of the other four equations. Another relationship is needed. This involves the temperature as measured by the brine RTD, per the argument given below.

The rate of heat transport within the brine/waste by natural convection is much greater than that by thermal conduction. This is borne out by the high Rayleigh Number, indicative of the ratio of these two heat-transport mechanisms, that exists in this region. Since natural convection dominates heat transport in the brine/waste, and since the radial heat transport in this region has been argued above to be relatively low, the *bulk* temperature in this recirculating region must be nearly isothermal, and thus well approximated by the brine/waste RTD measurement. A sketch of the probably axial temperature distribution in the brine/waste is shown in Fig. 15. It is also noted that in this one-dimensional model the heated and cooled surface areas of the brine/waste are both approximately equal to the test container interior cross-sectional area. Furthermore, the heat transfer at the lower brine region and heat transfer at the upper brine surface both involve higher temperatures underneath the interface of interest, so the heat-transfer coefficients should be comparable. Therefore, the temperature drops in the brine/waste at the lower and upper regions in the brine must be comparable. This argument is equivalent to forcing the *bulk* brine/waste temperature to be equal to the RTD measurement and at the arithmetic average temperature. With reference to the region and interface numbering shown in Fig. 14, T_3 (or T_2) can therefore be expressed in terms of the measured RTD temperature, T_{RTD} , from

$$T_{RTD} = \frac{T_2 + T_3}{2} \quad (58)$$

Only in the upper head and clamp region do multi-dimensional effects become significant. There, as depicted in Fig. 16, heat from the headspace is transported to the glovebox environment from both the upper and the cylindrical sides of the massive head and clamp assembly. The larger cross-sectional area and outer surface area contribute to a reduced resistance to heat flow from inside to the glovebox interior compared to the one-dimensional model. To account for this, two methods were used to determine an effective conductance, h_H , which, when used in the one-dimensional model, would yield approximately the same heat transfer rate as would occur in the actual geometry with the appropriate transport properties.

Fig. 15. Hypothesized Axial Temperature Distribution in the Brine/Waste

Fig. 16. Two-Dimensional Effects in the Test-Container Head Region

One method was to model the upper head and clamp regions carefully using the two-dimensional model previously described and impose a constant temperature on the inside surfaces of the vessel head. The heat flow rate to the fixed-temperature environment could then be equated to the heat-flow rate from the one-dimensional model having the same temperature beneath the head to determine an effective conductance value. This effect can be expressed as a multiplier on the normal transport properties of the head material. Instead of a constant factor, the factor varied somewhat depending on the temperature level because of the temperature dependency of the natural convection at the outer surface. These calculations found a typical multiplier factor of about 4.35, but are not exact because of the impressed uniform temperature assumption on the inner surface.

A second method involved computing an effective cross-sectional area for heat transport through the head. The second method requires only a knowledge of the geometry. The inner and outer surface areas of the head were simply averaged, and this value was divided by the one-dimensional cross-sectional area. This method found a multiplication factor of about 5.1. This calculation does not accurately account for the contact conduction resistances between head and clamp nor the actual head orientation insofar as surface conductances are concerned. As a result of these comparisons, the heat-transport coefficient for the head and the outer surface in the one-dimensional model were simply augmented by a factor of 5.0, and this factor was used consistently in all applications of the one-dimensional model.

A high Rayleigh number was also found to exist within the headspace-gas region. Again, this indicates that heat transport by conduction through the headspace gas is low compared to that transported by natural convection. So, by argument similar to that given above concerning heat transport in the brine/waste, the bulk gas temperature in the headspace must also be nearly uniform. Heat-transfer coefficients should be comparable over all of the boundaries of the headspace. However, the cylindrical surface around the headspace provides an additional cool-surface area for heat transfer that, together with the area provided by the underside of the head, is larger than the hot surface area (the surface of the brine). So although the isothermal assumption in the headspace remains valid, the *mean* headspace-gas temperature favors the cooler temperature of the underside of the container head closure instead of the average of the temperatures on the underside of the container head and on the brine surface. Ratioing the surface areas bounding the headspace cavity in the two-dimensional and one-dimensional models, the mean temperature is biased toward the temperature on the underside of the head by about 2:1. For example, if the brine surface were at 30°C and the underside of the test container head were at 15°C, the bulk headspace-gas temperature must be approximately 20°C. Mathematically, this relation is just

$$T_{HS} = T_1 + \frac{(T_2 - T_1)}{3} \quad (59)$$

Once the various heat-conductance coefficients have been evaluated the interface temperatures in the model, i.e., T_0 , T_1 , and T_2 , can be quickly found from Eqn. (56)–(58), allowing T_{HS} to be determined from Eqn. (59). It is noted, however, that three of the four conductance parameters involve natural convection. These are rather sensitive functions of temperature, requiring

iterative solutions to ensure that they are based on temperatures that are consistent with the final computed temperature distribution. Therefore, while conceptually simple, the actual solution of even the one-dimensional model becomes somewhat tedious. A comprehensive FORTRAN program was written and used. This program evaluated the conductance parameters using an assumed temperature distribution and then iterated the solution until satisfactory convergence was obtained. The entire thermal model program was then embedded as a subroutine in the overall analysis calculation program.

Table 3 lists the thermophysical properties and parameters selected for this application.

Table 3. Thermo-Physical Properties Used in the Thermal Model

	Temperature [C]	Thermal Conductivity [W/m/C]	Kinematic Viscosity [m ² /s ²]	Constant-Pressure Specific Heat Capacity [J/kg/C]	Mass Density [kg/m ³]
Glovebox Gas (Argon)	-23.16	0.0152	1.20E-05	520	1.630
	26.84	0.0177	1.69E-05	520	1.358
	126.84	0.0223	2.84E-05	520	1.019
Test-Container Head (Hastelloy-C)	25	12.6	--	--	--
Headspace Gas (Nitrogen)	-23.16	0.0222	7.78E-08	1038	200.4
	26.84	0.0260	1.08E-07	1041	167.0
	126.84	0.0325	1.79E-07	1046	124.9
Brine/Waste (Brine/ Water)	0	0.501	1.44E-06	3399	1244
	20	0.597	8.16E-07	3393	1233
	40	0.628	5.36E-07	3401	1222
	60	0.651	3.89E-07	3408	1210

As a final note, the thermal model is based on knowledge of the bulk temperature within the glovebox, T_{∞} , in the *immediate vicinity* of the test container head, i.e., the *local* glovebox temperature. The test-container heaters hold the brine/waste temperature above that of the ZPPR Cell unless the ZPPR Cell were to be hotter than the heater setpoint, which never occurred. Therefore, the local bulk temperature within the glovebox is always somewhere between the temperature of the brine/waste and that of the ZPPR Cell. This temperature difference was termed the “excess” temperature, i.e., excess over the glovebox RTD measurement.

There was, in fact, no actual measurement of the local glovebox temperature. This is because of the poor choice for placement of the glovebox RTD, which was directly adjacent to the glovebox wall and underneath the subfloor (see position in Fig. 7). This placement causes the instrument to actually measure some intermediate temperature between that of the bulk glovebox interior and the ZPPR cell. To take at least some account for this measurement error, an algorithm, based on some rather crude temperature mapping within the glovebox, was included in the thermal model to estimate the local glovebox temperature, T_{∞} . The algorithm used was a 2nd-order polynomial fit to the measurements of the excess temperature versus that measured by the glovebox RTD. The equation fit was generated using the Microsoft EXCEL-97 program. For glovebox RTD

temperature, T_{GB} , measurements in Celsius, the excess temperature was estimated from the relation

$$\delta T_{ex} = 0.0215T_{GB}^2 - 1.2975T_{GB} + 21.503 \quad (60)$$

The local glovebox temperature is then just the sum of T_{GB} and δT_{ex} . The temperature-mapping data from which this algorithm was deduced is described in Appendix C.

Equation (59) provides the headspace-gas temperature for each set of RTD and glovebox temperatures once the thermal model has been executed. Calculation of the thermal model at the reference conditions and at each data point enables the desired headspace-gas-temperature ratio, T_g/T_{g0} , to be computed.

8.2 Mechanical Generation of Heat

It may be noted that the preceding analysis has made no consideration of the thermodynamic effects on temperature in the headspace gas that result from compression or expansion. This is worth further consideration, because to the headspace gas the thermal expansion or contraction of the brine/waste, however small the magnitude of the volume change may be, seems like a piston performing mechanical work (algebraically) on the gas. Conservation of energy considerations from elementary thermodynamics show that this process should affect the gas pressure and temperature, even in the absence of any heat transfer between the gas and its surroundings. Figure 17 depicts this process.

Fig. 17. Mechanical Work of Compression (or Expansion) in the Headspace Gas

This work process would, indeed, cause temperature changes in the gas and be important in a *transient* treatment of the problem. But the quasi-steady analysis presented here is fully indifferent to the particular process(es) by which the new thermodynamic states are achieved. In other words, the new temperature of the gas will eventually return to precisely that temperature dictated by equilibrium considerations between the gas and its surroundings, no matter what other processes may have taken place.

Even though mechanical work considerations have no role in the present, quasi-steady-state, analysis, a better understanding of the test container's temperature response can be gained by exploring this further. The process considered is a simple compression of the headspace gas by the expanding brine/waste (caused by an increase in the brine/waste temperature). A "1st Law", or conservation of energy, statement for the process for the "closed" system (i.e., no mass flows crossing the boundary) shown in Fig. 17 is

$$dU = dQ - dW \quad (61)$$

The terms on the right-hand side of this equation are not properties of the thermodynamic state, but, instead, are process dependent. The quantity W is the work performed *by* the system (the headspace gas, itself, as depicted in Fig. 17), Q is the heat transfer *to* the system across the system boundary, and U is the internal energy. The change in the internal energy in the gas as the "piston" moves from position 1 to position 2 is

$$\Delta U = Q_{1-2} - W_{1-2} \quad (62)$$

The heat transfer, Q_{1-2} , must be determined from a thermal analysis as the gas goes from equilibrium state 1 to the new equilibrium state 2. The work performed *by* the system (headspace gas) *on* the piston (brine/waste), W_{1-2} , for a *reversible* (no parasitic losses such as turbulence) moving-boundary process in a closed system is just

$$W_{1-2} = \int_1^2 P dV \quad (63)$$

The internal energy of an ideal gas is a function only of its temperature. This fact with the definition of the specific heat capacity at constant volume, c_V , relates the change in internal energy over the process to the change in the temperature as

$$\Delta U = M_g c_V \Delta T \quad (64)$$

This equation can also be written in terms of moles, but the form above is more conventional. The term c_V is the average value over the temperature range of interest, and, for nitrogen at room temperature, has a value of about 7.08E-3 atm-litre/g/K.

Combining Equations (62) through (64) gives the temperature increase in the gas as

$$\Delta T = \frac{1}{M_g c_V} (Q_{1-2} - \int_1^2 P dV) \quad (65)$$

If the headspace gas were perfectly thermally insulated from its surroundings, i.e., insulated from the headspace walls and from the piston (brine/waste), there would be no heat transfer, so Q_{1-2} would be zero. Eqn. (64) indicates that there would nevertheless be a temperature change in the gas as a result of the mechanical work, as was stated at the beginning of this section. Furthermore, since P is positive and dV for the system (gas) is negative for the compression process being considered, the change in the temperature would be positive, i.e., the gas temperature would increase, as expected. An expanding brine/waste scenario implies that the brine temperature is rising, so it would follow that heat is probably also being transferred *to* the gas, i.e., Q_{1-2} would be positive. This is a rate-limited process, but does act to increase the value of ΔT , and accounts for the increasing entropy depicted in Fig. 17.

In the actual case there will always be heat transfer of whatever magnitude and direction is needed to achieve thermal equilibrium between the gas and its surroundings (the test container head and the brine/waste). Whether the mechanical work causes the gas temperature to momentarily under-shoot, over-shoot, or just equal the new equilibrium value will depend on the values of the specific parameters, such as c_V , V_{HS} , β , etc. It will be demonstrated in Section 9.1.7 that the parameters relevant to GGE cause gas temperature changes that result from mechanical work to be non-negligible and to somewhat *under-shoot* the equilibrium value. This means that the role of mechanical work in GGE is to assist in the rapid attainment of the equilibrium temperatures, shortening the transient period required for heat transfer with the surroundings to

achieve the new equilibrium state. This adds further confidence to the appropriateness of the quasi-steady analysis presented in this report.

9.0 Validation of the GGE Data

To demonstrate both the validity of the GGE data and the utility of the analytic methodology, the example that was discussed in Section 1.3 and shown in Fig. 1 and Fig. 2 is considered once again. The full temperature traces measured for this test container (TC-153) were shown in Fig. 8. At about data point no. 16000 the heater set point on this container was deliberately raised, producing the sharp temperature rise shown (this is the temperature rise that was shown on a greatly expanded time scale in Fig. 1.) Within about 12 h the RTD temperature within this test container increased 10.2°C, from 29.6°C to 39.8°C. There was only a small effect on the glovebox temperature from the increased heat load in the glovebox, as seen in the same figure. The pressure within the test container (see Fig. 2 and Fig. 9) increased during this event from 14.615 MPa (2119.7 psia) to 15.663 MPa (2271.7 psia) according to the data records. Some time after reaching the high temperature the heater was then reset (evidently, somewhat lower than the original setting) and the temperature (and pressure) dropped to below their initial levels, as evident in Fig. 1 and Fig. 8. Further manipulation of the heater controller eventually re-established the original conditions.

Attention here is focused only on the initial rise in the test-container temperature from 29.6°C to 39.8°C. Recall that the earlier consideration of only the direct temperature effect for this case (see Section 1.3) failed badly to predict the actual pressure rise. A viable explanation of the physical phenomena must be able to accurately predict the accompanying pressure rise induced by this simple step in the temperature. This temperature change was much larger than the temperature variations that occurred during the normal GGE operation. If the methodology presented here correctly handles this relatively large-scale event, it can be expected to perform well over all of the data. The calculation below uses the methods described in the preceding sections to predict the pressure rise.

9.1 Computation at a Specific Point

For the present example, select the reference point to be those conditions that existed at the initiation of the temperature excursion: test-container RTD temperature of 29.6°C, glovebox temperature of 20.6°C, and pressure of 14.615 MPa (2119.7 psia).

9.1.1 Temperature Ratio

The local temperature within the glovebox in the vicinity of the test container was estimated by the algorithm in Eqn. (60) to be 3.90°C in excess of the temperature measured by the glovebox RTD at the cited reference point. At these conditions, the one-dimensional thermal model estimates a mean headspace-gas temperature of 28.29°C. The vapor pressure (of water) at this gas temperature is 3.847 kPa (0.558 psia). At the conditions that occur at the peak of the temperature rise, the test-container RTD measured 39.8°C, the glovebox RTD measured 20.9°C, and the local temperature excess over the glovebox RTD measurement was estimated to be 3.76°C. At these conditions the mean headspace-gas temperature was found from the one-

dimensional thermal model (Section 8.1) to be 36.30°C. The vapor pressure for water at this gas temperature is 6.047 kPa (0.877 psia).

The ratio of temperatures within the headspace was therefore estimated to be

$$\frac{T_g}{T_{g0}} = \frac{36.30 + 273.15K}{28.29 + 273.15K} = 1.02658$$

It is recognized that the overall accuracy of the methodology certainly does not warrant six significant digits. These are shown in this section only to highlight the variation.

9.1.2 Compressibility Ratio

The Beattie-Bridgeman equation, Equations (52) through (55), with the mean gas temperature and pressure at the reference conditions, gives $z_0 = 1.02382$. The final pressure for this calculation is unknown, so a guess is required to calculate $z = z(P, T_g)$. After a new predicted pressure has been found, the process can be iterated by successive substitution, using that pressure to find an improved value for z , computing an improved pressure, etc. The convergence requires a few iterations, but is straightforward. To expedite this example, simply use the final measured pressure of 15.663 MPa (2271.7 psia) to compute the compressibility factor, giving $z = 1.03438$. So the compressibility ratio is found to be

$$\frac{z}{z_0} = \frac{1.03438}{1.02382} = 1.01032$$

9.1.3 Mass Ratio

From Eqn. (10), the ratio of headspace-gas mass is

$$\frac{N}{N_0} = \frac{N_0 + \Delta N}{N_0}$$

During this brief temperature excursion there were no samples withdrawn, nor were any calibrations made to the pressure transducer. The event is of sufficiently short duration that the quantity of any gases that may have been generated is fully negligible. Therefore, the headspace-gas mass could only have changed if the quantity of gas dissolved in the brine changed as a result of solubility variation from the new conditions. The increased brine temperature will lower the equilibrium concentration of dissolved gas, although the accompanying increase in pressure will tend to counteract this to some degree. Equations (22) through (26) provide the basis for evaluating the equilibrium gas-solubility effect. Eqn. (26) implicitly includes the quantity (moles) of liquid, so an iterative solution with the headspace volume determination is required to accurately quantify the mass ratio. A few iterations yields the solution.

Were there no variation in the gas solubility, the term ΔN would be identically zero, so the mass ratio before and after the step temperature increase would simply be unity. In accordance with the

discussion in Section 5.2.3, variation in the headspace-gas mass as a result of any solubility variation can be ignored. So, for this example, the headspace-gas mass ratio in this example simply has a value of unity:

$$\frac{N}{N_0} = 1$$

9.1.4 Headspace-Volume Ratio

Table 4 shows the temperature and pressure measurements taken during each of the four headspace-gas-sample measurements for this test container, along with the measured glovebox temperatures. For these measurements the temperatures were constant throughout the sampling event. The shaded portion of the table gives some quantities derived from these measurements. The equation number, or other reference that is the source of the calculation, is shown in parentheses for each column. These include the bulk headspace-gas temperature, as calculated for each sample event from the one-dimensional thermal model, the vapor pressure of water, calculated at the bulk headspace-gas temperature, and the compressibility factors for the initial and final conditions during the gas expansion. The headspace volumes at the prevailing measurement conditions are shown in the last column (see Sections 6.2.1 and 6.2.2).

Table 4. Raw Headspace Volume Measurements for TC-153^a

No. ^b	P_1 [MPa] (psia)	P_2 [MPa] (psia)	T_{RTD} [C]	T_{GB} [C]	T_{EX}^c [C] (60)	T_{HS}^d [C] (59)	P_v^e [kPa] (psia) (Ref. 1)	z_1 (55)	z_2 (55)	V_{HS} [ml] (46)
-02	15.100 (2190.1)	15.033 (2180.4)	29.80	22.1	3.27	28.66	3.930 (0.570)	1.026620	1.026275	741.71
-03	14.973 (2171.7)	14.905 (2161.8)	30.55	27.9	2.08	30.39	4.344 (0.630)	1.027114	1.026764	719.57
-04	14.927 (2165.0)	14.860 (2155.3)	30.60	28.6	2.05	30.60	4.392 (0.637)	1.027017	1.026675	731.83
-05	14.863 (2155.7)	14.795 (2145.9)	30.40	27.7	2.09	30.23	4.302 (0.624)	1.026444	1.026101	720.73

- Columns shown unshaded are measurements; those shaded are calculated values, with the source (equation number or reference) shown in parentheses.
- Measurement No. -01 was made at low pressure and therefore not included in table.
- T_{EX} is an estimate of the local environment temperature within the glovebox above that measured by the glovebox RTD (see Appendix D).
- Bulk headspace-gas temperature calculated from the one-dimensional thermal model.
- Vapor pressure of water calculated at the temperature of the headspace gas.

For the temperature step from 29.6°C to 39.8°C the average expansion coefficient, $\bar{\beta}$, for the brine is 0.383e-3°C⁻¹ (Fig. B6). Table 5 gives the brine expansion coefficient (from Fig. B6) and the headspace volumes adjusted to the reference conditions, calculated as shown in Eqn. (50). These are averaged, per Eqn. (51), to yield the best-estimate value of 730.27 ml at the reference conditions. The container volume is 7272 ml (Section 6.1.1). Therefore, the brine volume at the reference conditions, V_{l_0} , is 7272 - 730.27 ml or 6542 ml.

The linear expansion coefficient, μ , for the container has a value of 11.3e-6 C⁻¹ (Ref. 10). At the new conditions following the step temperature increase, Eqn. (41) gives the test container volume increase as

$$\begin{aligned}\Delta V_C &= V_{C_0} (e^{3\bar{\mu} \Delta T_{RTD}} - 1) \\ &= 7272 \text{ ml } (e^{3(11.3E-6 C^{-1})(39.8 - 29.6^\circ C)} - 1) \\ &= 2.52 \text{ ml}\end{aligned}$$

Table 5. Adjusted Headspace Volume Measurements for TC-153

Measurement No.	V_{HS-j} [ml] (46)	DT_{RTD-j} [C]	T_{RTD-j} ave [C]	β_{ave} [C ⁻¹] (Fig. B6)	V_{HS-0j} [ml] (50)
-02	741.71	0.20	29.70	0.374 E-3	742.20
-03	719.57	0.95	30.08	0.375 E-3	721.90
-04	731.83	1.00	30.10	0.375 E-3	734.28
-05	720.73	0.80	30.00	0.375 E-3	722.69
Sum	--	--		--	2921.08
Ave. (V_{HS-0})	--	--		--	730.27

The brine/waste volume increase, from Eqn. (43), is

$$\begin{aligned}\Delta V_l &= V_{l_0} (e^{\bar{\beta} \Delta T_{RTD}} - 1) \\ &= 6542 \text{ ml } (e^{0.383E-3 C^{-1}(39.8 - 29.6^\circ C)} - 1) \\ &= 25.61 \text{ ml}\end{aligned}$$

So the headspace volume increase (Eqn. (38)) is

$$\Delta V_{HS} = \Delta V_C - \Delta V_l = 2.52 - 25.6 = - 23.09ml$$

The headspace volume ratio then becomes

$$\frac{V_{HS_0}}{V_{HS}} = \frac{V_{HS_0}}{V_{HS_0} + \Delta V_{HS}} = \frac{730.27ml}{730.27ml - 23.09ml} = 1.03265$$

9.1.5 Predicted Pressure

With the ratios determined in the preceding sections, the predicted total pressure following the temperature step change can be immediately computed from Eqn. (7):

$$\begin{aligned} P - P_v &= (P - P_v) \left(\frac{z}{z_0} \right) \left(\frac{N}{N_0} \right) \left(\frac{V_{HS_0}}{V_{HS}} \right) \frac{T_g}{T_{g_0}} \\ P - 6.047kPa &= (14.615MPa - 3.847kPa)(1.01032)(1.0)(1.03265)(1.02658) \\ &= 14.611MPa \cdot 1.07104 \\ &= 15.649MPa \quad (2269.7psia) \end{aligned}$$

So the predicted total pressure, i.e., the gas pressure plus vapor pressure, is

$$P = 15.649MPa + 6.047kPa = 15.655MPa \quad (2270.6psia)$$

This is quite close to the measured value of 15.663 MPa (2271.7 psia).

The relative contribution of each of the thermodynamic terms to the pressure rise can be quickly assessed for this example by examining the pressure calculation. Each of the four thermodynamic ratios has a value of unity or exceeds unity. The excesses, summed, exceed unity by a total of 0.06955. The headspace volume ratio is seen to be the biggest contributor to the pressure rise. This term contributes 0.03265/0.06955, or about 47% of the total excess, substantially greater than the 0.02658/0.06955, or 38%, contribution from the headspace-gas temperature. The compressibility variation contributes the remaining 15%. Recall that the volume ratio was the consequence of the thermal expansion of the brine/waste, lessened somewhat by the simultaneous thermal expansion of the test vessel, Eqn. (38). Little wonder then, that the earlier analysis of the data that considered only the direct temperature effect (*even when aided by the erroneous assumption that the headspace-gas temperatures were the same as those measured by the test-container RTD*) had failed so badly to predict the system response.

This computation demonstrates the validity of the GGE data. The remainder of this chapter further clarifies the calculation methodology.

9.1.6 Compensated Pressure

The treatment shown in the preceding section is a *predictive* form of the calculation: the original pressure and the variations of temperature and headspace-gas mass were used to predict the new pressure following some change. An alternate, but fully equivalent, point of view is to start with the actual final pressure measured and then purge that value of the effects of the temperature and/or headspace-gas-mass variations. With this approach, these effects will have been factored out, yielding an estimate of the original pressure. This approach is referred to in this report as the *compensated-pressure* form of the methodology. The compensated value provides an estimate of the reference pressure when there is no gas generation. As before, terms with zero subscript refer to the reference conditions, others refer to the new conditions following the temperature step. From Eqn. (8) and the values obtained in Section 9.1.5, the compensated pressure for the example becomes

$$\begin{aligned}
 P_{comp} - P_{v_0} &= (P - P_v) \left(\frac{z_0}{z} \right) \left(\frac{N_0}{N} \right) \left(\frac{V_{HS}}{V_{HS_0}} \right) \left(\frac{T_{g_0}}{T_g} \right) \\
 P_{comp} - 3.847 \text{ kPa} &= (15.663 \text{ MPa} - 6.047 \text{ kPa}) \frac{1}{1.01032} \frac{1}{1.0} \frac{1}{1.03265} \frac{1}{1.02658} \\
 &= (15.657 \text{ MPa}) \frac{1}{1.07104} \\
 &= 14.618 \text{ MPa} \quad (2120.2 \text{ psia})
 \end{aligned}$$

So the compensated total pressure is found to be

$$P_{comp} = 14.622 \text{ MPa} \quad (2120.7 \text{ psia})$$

As expected, this compares favorably to the actual pre-step (in this case the reference value) pressure of 14.615 MPa (2119.7 psia).

The above form of the example demonstrates the capability of the analytical methodology to reasonably accurately *recover* the original pressure of 14.615 MPa (2119.7 psia) after *compensating* the measured pressure for, i.e., nullifying, the effects of temperature variation. Comparing the P_{comp} expression above to the adjusted pressure P_{adj} defined in Eqn. (28), it is seen that P_{adj} and P_{comp} are exactly the same.

9.1.7 Mechanical Work

The role of mechanical-energy conversion on the headspace-gas temperature was discussed in Section 8.2, and can be demonstrated by this example. The headspace volume change was calculated in Section 9.1.4 to be -23.09 ml. With the cross-sectional area of the test container, 181.1 cm^2 , the displacement of the brine surface resulting from the brine expansion would have been only 1.3 mm. However, a force of approximately 274,680 N (61,750 lbf) must be exerted to displace the brine/waste surface against the high gas pressure that prevails.

For illustration purposes, the integral in Eqn. (65) is simply approximated by using the average pressure, and the headspace-gas mass is written using the state equation. Then the temperature rise, DT_{ME} , that results from the conversion of mechanical energy (alone) to internal energy for an adiabatic process is

$$\Delta T_{ME} = - \frac{1}{M_g c_v} \int_1^2 P dV \approx - \frac{z_0 R_U T_{g_0}}{P_{g_0} V_{HS_0} c_v [MW]} P_{ave} \Delta V_{HS} \quad (66)$$

The values for each of these terms from the previous example are substituted and the thermodynamic properties appropriate to nitrogen at room temperature are used:

$$\begin{aligned} z_0 &= 1.0238 \\ T_{g_0} &= 28.29 + 273.15 = 301.44 \text{ K} \\ \Delta V_{HS} &= - 23.09 \text{ ml} \\ V_{HS} &= 730.07 \text{ ml} \\ P_{ave} &= 0.5(14.615 + 15.663) \text{ MPa} = 15.139 \text{ MPa} \text{ (2195.7 psia)} \\ R_U &= 0.08206 \text{ atm-litre/g-mole/K} \\ c_v &= 7.08E-3 \text{ atm-litre/g/K} \\ [MW] &= 28 \text{ g/(g-mole)} \end{aligned}$$

Therefore, the mechanical work performed in compressing the headspace gas is found to raise the gas temperature approximately 4.13°C. This calculation over-estimates DT_{ME} somewhat, because the average pressure in Eqn. (66) was calculated using the final pressure, not just that portion of the pressure increase that resulted from the mechanical compression. The actual value can be found from the thermodynamic relations for the isentropic compression implied in this example. For such a process in an ideal gas, PV^g is a constant. For the same ΔV_{HS} , this shows that the mechanical compression, alone, causes the pressure to increase to 15.301 MPa (2219.2 psia). The temperature rise from the mechanical work is found to be about 4.08°C.

This is the temperature rise that would occur *if* the 23.09 ml compression of the headspace gas had occurred adiabatically. Heat transfer from the brine/waste to the headspace gas and then out to the glovebox environment provides the further temperature increase to the final equilibrium temperature of 36.30°C, i.e., a total temperature rise of 36.30 - 28.29°C = 8.01°C.

9.2 Adjustment of the Pressures in the Blank, Experiment-Control Test Containers

The adjusted pressure was computed for each data point for the two non-waste-bearing test containers, No. 152 and 153. The calculations required and made at each data point are the same as that shown in the example in Section 9.1. These are relatively simple calculations, but the plethora of data points and the several iteration routines that are required dictated the use of the

computer program. The final evolution of the special program developed, *GGE7b1*, is described in Appendix D. Temperature and pressure measurements were taken hourly, yielding approximately 26,000 data points for each test container over the more than three years of data considered in this report. Each of these data points were processed to provide the results presented here.

The computation was begun by appending to each point in the data file an estimate of the local glovebox temperature per the algorithm described in Eqn. (60). The FORTRAN computer program reads this data file, and, using the methods described in Sections 5.0 through 8.0 of this report, determines the thermodynamic-parameter ratios needed to evaluate the adjusted pressure from Eqn. (28). The adjusted pressures are written to an unformatted-text output file, which, for convenience, is subsequently inserted into a Microsoft EXCEL program. The change in mole fraction of the generated gases relative to the reference point, dX_{gen} , is calculated from Eqn. (33) and added to the spreadsheet. Finally, the adjusted pressures and mole fractions are plotted using the spreadsheet plotting utility.

Figure 18 and Fig. 19 show the temperatures for the two blank test containers, TC-152 and TC-153. The points at which headspace-gas samples were taken are marked on the figures, as are the points at which RTD calibration checks were made. Figure 20 and Fig. 21 show the corresponding pressure data. Superimposed on the measured pressure plots are the adjusted pressures as computed by the *GGE7b1* FORTRAN program. These are relative to the arbitrarily selected reference point identified in the title line on each plot. The points at which headspace-gas samples were extracted and the pressure-instrument calibrations made are shown on the pressure plots. The drop in pressure of approximately 55–70 kPa (8–10 psi) that occurred each time a headspace gas sample was drawn is evident in the pressure data record.

Fig. 18. Temperatures, TC-152

Fig. 19. Temperatures, TC-153

Fig. 20. Pressures, TC-152 (Ref. Pt. 10001)

Fig. 21. Pressures, TC-153 (Ref. Pt. 10001)

The computed adjusted-pressures for both blank test containers show an approximately constant value, as anticipated, and the pressure rise that occurred at the temperature spike addressed earlier in this section is duplicated by the program. The variation from a constant value is modest, and this variation is indicative of the uncertainty that must be accepted when using the analysis methodology on field data. Considering the plethora of uncertainties and assumptions imbedded in the data-recovery methodology, the results are satisfactory. Imperfections inherent in the methodology are discussed in Section 13.0. Notwithstanding these inherent imperfections, the adjusted pressures for these two test containers are the actual pressures that would have prevailed had there been no temperature variation in the headspace gas nor any changes to the headspace-gas masses from sampling or PXD calibrations. The adjusted pressure plots reveal the pressure variation that remains after analytical compensation for the headspace temperature and mass changes.

The mole fractions of generated gases over the experiment are depicted in Fig. 22 and Fig. 23. The mole fraction traces also, of course, reflect the imperfections in the analysis and any discrepancies that are imbedded in the data, but it is quite clear that there are no perceptible indications of long-term gas-generation trends.

Fig. 22. Gas Generation in TC-152

Fig. 23. Gas Generation, TC-153

10. Recovery of the Archived Pressure Measurements

The previous section established both the validity of the experimental data as well as the usefulness of the analyses. Attention is now turned to recovering the extensive data that was collected during the first 3.25 years of the experiment. This requires a slight modification to the methodology. The key new features are described in this section.

10.1 Determination of the Brine/Waste Thermal Expansion Coefficient

The calculations in Section 9.0 were made using a value for the brine expansion coefficient that was determined from dedicated measurements made on the brine in a separate experiment (Appendix B). Analogous measurements were not made, and are probably not possible to make with any reasonable accuracy, for the various brine/waste combinations. To do so would require duplicating the brine/waste in the off-line experiments. Not only would this be costly and time consuming, there is little likelihood that the physical arrangement of these mixtures could be duplicated to provide meaningful data. For example, bubbles trapped within the waste matrix play a profound role in the overall “elasticity” of the material, and duplication of the bubble quantity and distribution that may be in the actual test containers would be impossible.

A different approach was needed, and the one devised was, in fact, much simpler. A step temperature change was deliberately introduced into each test container’s heater controller. This was limited to one or two test containers at a time, so as to not significantly affect the overall glovebox heat load. The system was not further disturbed for the 3-4 days required to ensure the establishment of a new equilibrium operating point. The test-container temperature and corresponding pressure response were then duly measured and recorded. This provided data

similar to the incidental temperature spike that was addressed in the data-validation example in Section 9.1. Based on the experience found in the validation examples, an accurate value for the brine/waste expansion coefficient, β , would be expected to yield an accurate prediction of the adjusted pressure response. Now, instead of applying the analyses to predict the pressure response, the measured response, itself, was used to back the brine/waste expansion coefficient out of the analyses. That is, the predicted pressure for the induced temperature spike was forced to match the measured response, allowing the value of β to be determined from the analyses. Once this parameter was obtained from the measured pressure response to the induced temperature step, it could then be used with the entire set of archived data for that test container to calculate the adjusted pressures at all other data points.

The analytical development for this approach is as follows. Let subscript “1” refer to the conditions just prior to the induced temperature step, and subscript “2” refer to the new equilibrium conditions following the step. Equations (36) through (38) relate the headspace volume following the step to that just before the temperature step as

$$V_{HS_2} = V_{HS_1} + \delta V_{C_{step}} - \delta V_{L_{step}} \quad (67)$$

Similar to Eqn. (41) and (43), expressions for $\delta V_{C_{step}}$ and $\delta V_{L_{step}}$, respectively, can be derived for the conditions of the step change in the headspace volume.

From Eqn. (41),

$$\delta V_{C_{step}} = V_{C_1} (e^{3\bar{\alpha}_{step}\delta T_{step}} - 1) \quad (68)$$

The subscript “*step*” emphasizes that the associated terms refer specifically to the changes that occur between the pre- and post-induced-step conditions, i.e., over the transition from state 1 to state 2. For example, this report generally uses DT_{RTD} to refer to the difference between the container RTD temperature (i.e., brine/waste temperature) at the current point minus the RTD temperature at the reference point. When the lower-case delta symbol (δ) is used it refers simply to some change. For the specific case where the variable is subscripted *step*, it refers to the step conditions (the value after the step minus the value just prior to the step. Were the reference point always taken at the pre-step conditions, there would obviously be no difference in the nomenclature; however, it is preferred to keep this development general, allowing the reference point for the overall calculation to be arbitrarily selected independently of the induced step measurements.

The container volume at the pre-step conditions can be related back to the corresponding volume at the overall reference point by using Equations (39) and (41) to obtain

$$V_{C_1} = V_{C_0} e^{3\bar{\alpha}_{1-0}\Delta T_{1-0}} \quad (69)$$

The subscript here emphasizes that the terms refer to the interval or difference from the pre-step conditions to the overall reference point. This relation can be substituted into Eqn. (68) to find the change in container volume when referenced to the volume at the overall reference point.

Similarly for the brine/waste, from Eqn. (43), $dV_{l\text{-step}}$ becomes

$$\begin{aligned}\delta V_{l_{step}} &= V_{l_1}(e^{\bar{\beta}_{step}\delta T_{step}} - 1) \\ &= (V_{C_1} - V_{HS_1})(e^{\bar{\beta}_{step}\delta T_{step}} - 1)\end{aligned}\quad (70)$$

The headspace volumes at the conditions both before and following the step can be written using the equation of state:

$$V_{HS} = \frac{zNR_U T_g}{P_g} \quad (71)$$

Upon combining Equations (67) through (71) and rearranging, the average value of the expansion coefficient over the step, β_{step} , is found to be

$$\beta_{step} = \frac{1}{\delta T_{step}} \log_e \left(\frac{V_{C_0} e^{3(\bar{\alpha}_{1-0}\Delta T_{1-0} + \bar{\alpha}_{step}\delta T_{step})} - \frac{z_2 N_2 R_U T_{g_2}}{P_{g_2}}}{V_{C_0} e^{3\bar{\alpha}_{1-0}\Delta T_{1-0}} - \frac{z_1 N_1 R_U T_{g_1}}{P_{g_1}}} \right) \quad (72)$$

There is a temperature dependency for the β term. This is evident from Fig. B6 in Appendix B for tests conducted on pure brine, as well as for pure water shown in Fig. B5; hence, the inclusion of the average value in Eqn. (70) (note that Eqn. (68) has also been developed for the general case of a temperature-dependent α , although a constant value of $11.3\text{e-}6\text{ C}^{-1}$ was used in all of the calculations in this report). For this reason, two separate step temperature changes were actually induced in each test container: a “high-temperature” step, obtained by increasing the test-container-heater set point well above the normal operating temperature; and a “low-temperature” step, obtained by reducing the heater set point to below the normal-operating level. The maximum permissible temperature was 40°C to avoid harming the inoculated microbes (15). An equation like that above was written for both the high-temperature and low-temperature steps. In the high-temperature-step equation, the average value of β over the temperature step is denoted as β_H , while for the low-temperature step the average value is denoted β_L . Solutions to these equations yield two fixed values for β that cover the temperature range of interest. Having determined these two values, the actual temperature-dependent value for β at any temperature, T_{RTD} , inbetween was expressed as a linear function of β_H and β_L ,

$$\beta = \beta_L + (\beta_H - \beta_L) \frac{T_{RTD} - T_{RTD_L}}{T_{RTD_H} - T_{RTD_L}} \quad (73)$$

Equation (72) cannot be solved explicitly, however, because the derived headspace-gas masses in the equation, N_1 and N_2 , are, themselves, functions of β . This is shown in the following development.

The mass at state 2 is related to the mass at state 1 by

$$N_2 = N_1 + \delta N_{step} \quad (74)$$

where, as discussed in Section 5.2,

$$\delta N_{step} = \delta N_{sampling} + \delta N_{pxd} + \delta N_{sol} + \delta N_{gen} \quad (75)$$

There are no gas samples or pressure-transducer calibration events that occur between the current point and the reference point. And since the time frame is so short,

$$\delta N_{step} = \delta N_{solubility} + \delta N_{generation} \approx 0 \quad (76)$$

The headspace-gas mass remains approximately constant during the step event, and the value can be related back to that at the overall reference point by using

$$N_2 = N_1 = N_0 + \Delta N_{1-0} \quad (77)$$

As before, in Eqns. (18) and (21), the change in mass relative to that at the reference point can be written as

$$\Delta N_{1-0} = \mp \left(\sum_{i=1}^J \delta N_{D_i} + \sum_{i=1}^K \delta N_{C_i} \right) \quad (78)$$

Calculations of the various dN terms were discussed in Section 5.0. The headspace-gas mass at the reference point must be computed from the equation of state,

$$N_0 = \frac{P_{g_0} V_{HS_0}}{z_0 R_U T_{g_0}} \quad (79)$$

Alas, it is recalled from Section 6.2.2 that the calculated headspace volume at the reference point, i.e., V_{HS-0} , is the average of the adjusted measurements made during sampling. These adjustments, per Eqn. (50), clearly depend on the value of β .

Given the transcendental character of Eqn. (72), the solution was obtained by iteration, using successive substitution. A mean headspace volume at the reference conditions, V_{HS-0} , was first

guessed and used in Eqn. (79). This allowed the headspace-gas mass at the step conditions to be found from Equations (77) and (78). Then the values for β_H and β_L were computed from the step relation, Eqn. (72). With these two values and Eqn. (73), the appropriate values of β for each of the sample measurements could be computed allowing the raw headspace-volume measurements to be adjusted to the reference conditions per Eqn. (50). Then a new average headspace volume at the reference conditions was computed, Eqn. (51), and substituted back into Eqn. (79) to improve the headspace-gas mass value. The process was repeated until the reference headspace volume converged per some pre-selected convergence criterion.

Even with an extremely poor starting guess for the reference headspace volume, the solution was found to converge rapidly. For example, a relative error of less than one part in 10,000 could be obtained in just 4 or 5 iterations. The iteration process was built into the overall analysis program and was performed automatically. Once β_H and β_L were determined, the value of β at the required temperature could be computed from Eqn. (73) for use in the analysis of each data point.

This process was performed for each test container, yielding a temperature-dependent equation for β that was unique to each container, i.e., unique to the brine/waste mixture within each test container. The expansion coefficients so determined are listed in Table 6.

Table 6. Volumetric Coefficients of Thermal Expansion in the Brine/Waste

Test Container No.	T _{RTD-L} [C]	Beta-L [C ⁻¹]	T _{RTD-H} [C]	Beta-H [C ⁻¹]
TC-151	27.3	1.98E-4	33.8	2.35E-4
TC-152	28.1	3.71E-4	35.6	3.74E-4
TC-153	27.7	3.62E-4	34.7	3.67E-4
TC-160	27.1	3.68E-4	33.6	3.51E-4
TC-161	27.2	3.69E-4	32.9	3.75E-4
TC-161e^a	27.2	3.70E-4	33.0	3.77E-4
TC-162	28.2	3.88E-4	33.8	3.88E-4
TC-163	27.9	4.03E-4	33.9	3.83E-4
TC-164	27.3	3.94E-4	33.9	3.82E-4
TC-165	27.7	3.64E-4	32.6	3.83E-4
TC-166	27.2	3.43E-4	32.9	3.39E-4
TC-167	28.6	3.46E-4	33.1	3.58E-4
TC-168	27.5	3.57E-4	33.3	3.75E-4
TC-169	27.8	3.67E-4	33.9	3.81E-4
TC-170	30.6	3.28E-4	32.8	3.57E-4

a. TC-161e uses empirical calibration constants for TC-161, per discussion in Section 11.2.1.

10.2 Instrument Calibrations

Regular calibration checks were made to the instruments and recorded as part of the GGE program. When calibration errors in excess of a specified threshold were detected, the instrument was adjusted. The analyses reported here accounted for all calibration corrections that had been made by assuming these to have been the result of a steady, uniform deterioration of the accuracy since the previous calibration check.

Consider an instrument that was perfectly calibrated when checked at time t_1 , and some time later, say at time t_2 , a new calibration check found that the instrument was out of calibration by an amount d_{cal} (whether the adjustment was actually made to the instrument channel, or not). Each data point collected with this instrument between t_1 and t_2 was corrected in the analysis methodology on the basis of an assumed uniform degradation over the interval. For example, the data in this time interval at arbitrary time t was linearly corrected by an amount

$$\delta_{correction} = \delta_{cal} \frac{t - t_1}{t_2 - t_1} \quad (80)$$

Instrument adjustments were made when the calibration error exceeded a pre-selected threshold. The calibration check was then repeated. If the calibration check showed the instrument to be operating within the allowable bounds (either the initial calibration check or that made following any adjustment) no further adjustment was made. Any residual error, however, was noted in the operation logs. These residuals then were applied to data acquired during the next interval prior to the next calibration check.

The corrections were algebraically added to the data point prior to processing the point with the analysis program. This type of data-correction was implemented for both temperature and pressure data. The calibration corrections were included in all of the adjusted pressure calculations shown in this report, including those in Section 9.2, although in only one case, discussed in Section 11.2.1, was it ever a significant factor in any of the results.

11. Recovered Data

Recovery of the GGE data for a given test container consisted of computing the adjusted pressure, Eqn. (28), from measurements of the pressure, brine/waste RTD temperature, and glovebox temperature that were recorded at each data point. The adjusted pressure was then used to compute the change in the mole fraction of generated gases, via Eqn. (32). These results are presented pictorially and discussed in this section.

11.1 Analysis Results

Figure 24–Fig. 35 show the temperatures, adjusted pressures, and mole fractions of generated gases for each of the twelve waste-bearing test containers in the GGE program. Three plots are shown for each test container. Figure numbers with a *A* suffix are plots of temperatures. The corresponding plot for pressure carries the same figure number, but with a *B* suffix; and the mole

fraction of generated gases for the same test vessel has a *C* suffix. Figures 24–Fig. 35 correspond to Test Container No. 151 and 160 through 170, respectively. Similar results for Test Containers No. 152 and 153 were presented in Fig. 18–Fig. 23 and discussed in Section 9.2. Every valid data point has been treated in each of these plots. No filtering has been applied to either the data or to the adjusted pressures.

The temperature plots, Fig. 18 and Fig. 19, and Fig. 24 through Fig. 35, suffix *A*, show the measurements made by resistance temperature detectors in the test container and in the glovebox. A third, intermediate, temperature trace labeled “Estimated Local TC Environment” is the estimate of the glovebox temperature in the immediate vicinity of the test container, as was discussed in Section 8.1. These plots clearly show when the test container temperatures are being dictated by the local glovebox temperature. Headspace-gas sampling points and instrument calibrations are marked on these temperature plots. It is also clear that the algorithm, Eqn. (60), used to estimate the local test-container environment is better suited to some of the test containers than to others. For example, the estimated local environment for TC-152 (Fig. 18) tracks the brine/waste temperature very well, whereas the estimated local environment for TC-161 (Fig. 26A) doesn’t fit quite as well. The fit of the algorithm to the other test containers lay inbetween these two. This probably results from the influence of other nearby equipment and/or flow patterns both within and outside of the glovebox.

The adjusted pressures, calculated per the analysis developed in this report, are superimposed on the pressure-data (suffix *B*) plots. Calculations for the 3.25 year period from the beginning of the tests through the end of May 1999 are provided. These figures also show the points at which the pressure instrumentation was calibrated and when headspace-gas samples were taken.

Fig. 24A. Temperatures, TC-151

Fig. 24B. Pressures, TC-151 (Ref. Pt. 10001)

Fig. 24C. Gas Generation in TC-151

Fig. 25A. Temperatures, TC-160

Fig. 25B. Pressures, TC-160 (Ref. Pt. 10001)

Fig. 25C. Gas Generation in TC-160

Fig. 26A. Temperature, TC-161

Fig. 26B. Pressures, TC-161 (Ref. Point No. 10001)

Fig. 26C. Gas Generation in TC-161

Fig. 27A. Temperatures, TC-162

Fig. 27B. Pressures, TC-162 (Ref. Point No. 10001)

Fig. 27C. Gas Generation in TC-162

Fig. 28A. Temperatures, TC-163

Fig. 28B. Pressures, TC-163 (Ref. Point No. 10001)

Fig. 28C. Generated Gas, TC-163

Fig. 29A. Temperature, TC-164

Fig. 29B. Pressure, TC-164 (Ref. Point No. 10001)

Fig. 29C. Gas Generation in TC-164

Fig. 30A. Temperatures, TC-165

Fig. 30B. Pressures, TC-165 (Ref. Point No. 10001)

Fig. 30C. Gas Generation, TC-165

Fig. 31A. Temperatures, TC-166

Fig. 31B. Pressures, TC-166 (Ref. Point No. 10001)

Fig. 31C. Gas Generation, TC-166

Fig. 32A. Temperatures, TC-167

Fig. 32B. Pressures, TC-167 (Ref. Point No. 10001)

Fig. 32C. Gas Generation, TC-167

Fig. 33A. Temperatures, TC-168

Fig. 33B. Pressures, TC-168 (Ref. Point No. 10001)

Fig. 33C. Gas Generation, TC-168

Fig. 34A. Temperatures, TC-169

Fig. 34B. Pressures, TC-169 (Ref. Point No. 10001)

Fig. 34C. Gas Generation, TC-169

Fig. 35A. Temperatures, TC-170

Fig. 35B. Pressures, TC-170 (Ref. Point No. 10001)

Fig. 35C. Gas Generation, TC-170

11.2 Discussion

11.2.1 Adjusted Pressure Results

The adjusted-pressure results were generally found to be satisfactory. As was pointed out before, there are numerous uncertainties, parameters, properties, and other aspects that can effect the accuracy of the calculations. These are discussed in Section 13.0. The most suspect adjusted pressures for all of the test containers occurred during the period immediately following the first activation of the ZPPR air-conditioning system on October 22, 1997 (Point 2 on Fig. 8) to alleviate the elevated, summertime temperature in the ZPPR Cell. This rather sudden reduction in the ZPPR-Cell temperature also caused a near-simultaneous drop in the GGE glovebox temperature of about 10°C.

A possible explanation for the less satisfactory behavior of the adjusted pressures during this period is that the sudden cooling of the glovebox probably caused all of the test-container heaters to be simultaneously energized. This would have caused the “local excess temperature” to deviate drastically from that mapped later, when temperatures had largely stabilized at earlier conditions. This would imply that the algorithm, Eqn. (60), used in the calculation to compute the local excess temperatures during this period may have been less appropriate during this period.

The adjusted pressure calculated for Test Container No. 161 is obviously the least satisfactory of all of the test containers. For this test container there is a notable lack of continuity overall in the adjusted pressure slope. Over the intervals *between* the discontinuities, the adjusted pressures behave quite well. The discontinuities all occurred precisely at the points where the

test-container RTD instrument calibrations were performed, as marked in Fig. 26B. This observation prompted a closer scrutiny of all of the calibration data, for which a few ambiguities had been noted earlier in the operations logs.

A purely empirical process was explored for Test Container No. 161 to determine if RTD-calibration corrections, alone, could be responsible for the bizarre behavior of the adjusted pressure. Per the discussion in Section 10.2, it is relatively easy to foresee how instrument-calibrations factors (both adjustments and residual errors) will affect the adjusted pressure. Figure 36 shows the temperatures for Test Container No. 161 using the combination of RTD calibration factors that would yield the best behaved adjusted pressure. These temperatures are nearly identical to those shown in Fig. 26A. The pressure is shown in Fig. 37. It is clear from Fig. 37 that the discontinuities at the RTD-calibration points have been largely eliminated, lending support to the concern that, although unexplained, errors were introduced in the calibration records for this test container. Table 7 provides a comparison of the recorded calibration factors versus those empirically determined to best eliminate the bothersome characteristics in the adjusted-pressure results for TC-161. However, no definitive resolution could be reached as to why such records for this test container would have been more affected than calibration records for the other test containers.

Fig. 36. Temperatures, TC-161 - Empirical RTD-Calibration Corrections

Fig. 37. Pressures, TC-161 (Ref. Point No. 10001) - Empirical RTD-Calibration Corrections

Fig. 38. Gas Generation in TC-161 - Empirical RTD Calibration Corrections

Table 7. Comparison of RTD Calibration Corrections for TC-161:
Recorded (TC-161) versus Empirical (TC-161e) Corrections

Date	Data Pt. No.	Recorded Adjustment [C]	Recorded Residual [C]	Empirical Adjustment [C]	Empirical Residual [C]
02-12-96	1	0.	0.	0.	0.
07-15-96	3323	0.5	0.	0.8	0.
01-13-97	7558	0.	0.	0.3	-0.1
07-09-97	11626	0.	0.1	-0.35	0.45
11-21-97	14848	0.6	0.1	0.6	0.
05-21-98	19142	-0.9	0.	-0.7	0.7
11-21-98	23524	0.4	0.	0.6	-0.1
05-25-99	27711	0.	-0.1	0.1	0.

11.2.2 Examination for Evidence of Gas Generation

Figures 24 through Fig. 38, suffix C, show the mol fractions of generated gases for Test Containers No. 151 and 160 through 170, respectively, relative to the mol fraction at the indicated reference conditions. Similar gas-generation results for the two test blanks, Test Containers No. 152 and 153, were presented in Section 9.2, Fig. 22 and Fig. 23.

Examination of these figures quickly identifies the test containers in which significant gases are being generated. These are Test Containers No. 151, 160, 161, 166, and 167. Some lesser rates of gas generation might also be perceived in Test Containers No. 162 and 163. There was either no or negligible perceptible gas generation over the 3.25 year test period through May 1999 for the other test containers. Rates of gas generation, inferred per Eqn. (35) by visual examination of the figures, are given in Table 8. The gas-generation results for Test Container No. 161 (Fig. 38) were based on the adjusted pressure recomputed using the empirical RTD-calibration corrections discussed in the previous section and shown in Table 7.

Test Container No. 166 shows a considerably higher gas-generation rate than any of the others. Gas generation seems to have been modest for the initial 9.5 months, but then began at a rather high rate. Omitting the initial period, i.e., prior to about Data Point No. 6001, gases are apparently being generated in Test Container No. 166 substantially faster than in the other gas-generating test containers during the period covered in this report.

Since the objective of this report is only to document the analytical process by which the pressure data was resolved and recovered, further analysis of the gas-generation results is deferred to other GGE program reports.

Table 8. Graphically Inferred Gas-Generation Rates

Test Container No.	Point-b Point No.	Point-b Date	Relative Mol Fraction $DX_{\text{gen-b}}$	Point-a Point No.	Point-a Date	Relative Mol Fraction $DX_{\text{gen-a}}$	Elapsed Time Interval, t [days: years]	dX_{gen}	dX_{gen}/dt [ppm/yr]
151	12501	11-17-97	0.0015	4501	12-08-96	-0.0015	344: 0.942	0.0030	3183
152	11501	10-19-97	0.0000	5501	02-03-97	0.0000	258: 0.707	0.	0
153	23501	03-19-99	-0.0018	14501	02-25-98	-0.0018	387: 1.060	0.	0
160	12501	09-26-97	0.0015	4501	10-17-96	-0.0033	344: 0.942	0.0048	5096
161e	24501	01-08-99	0.0040	10501	05-23-97	0.0000	595: 1.630	0.0040	2454
162	23501	12-07-98	0.0007	4001	08-27-96	-0.0008	832: 2.279	0.0015	658
163	23001	11-29-98	0.0010	5001	10-20-96	-0.0005	770: 2.110	0.0015	711
164	22501	11-19-98	0.0002	6501	01-02-97	-0.0005	686: 1.879	0.0007	373
165	23001	12-07-98	0.0000	5001	10-28-96	-0.0005	770: 2.110	0.0005	237
166	24501	03-04-99	0.0110	16001	02-22-98	0.0030	375: 1.027	0.0080	7790
167	23501	01-17-99	0.0035	4001	10-03-96	-0.0020	836: 2.290	0.0055	2402
168	12501	10-07-97	0.0000	6001	10-06-96	0.0000	366: 1.003	0.	0
169	22001	11-26-98	-0.0003	4001	10-20-96	-0.0003	767: 2.101	0.	0
170	21501	11-27-98	-0.0008	15501	03-17-98	-0.0008	255: 0.699	0.	0

12.0 Applicability to Other Investigations and Experiment-Design Implications

The GGE program consistently maintained the test containers well within the $\pm 5^\circ\text{C}$ experiment specifications for temperature. Nevertheless, the pressure data collected in the ANL GGE program was found to be unusable without the compensation methodology described in this report, and it was clearly established that even the very small temperature variations that did occur were the primary contributor to the pressure fluctuations observed. The question arises as to whether other gas-generation experiments have experienced similar pressure behavior, and, if not, why not? The answer to this question is discussed in this section, and provides useful guidance to the design of future experiments.

The GGE program used very prototypic conditions. The pressure was selected to match the very high lithostatic pressure expected eventually at WIPP, and waste compositions, packing, and radioactivity levels were typical of those TRU wastes destined for WIPP. These conditions are key to the following discussion.

Equation (2) shows how the pressure, temperature, mass, and volume at a given state are related. Assume that in the vicinity of a given set of operating conditions the compressibility, z , and the headspace-gas mass, M , are constant. Then the pressure variation induced by variations in temperature or headspace-gas volume can be found by differentiating Eqn. (2), giving

$$dP = zMR \frac{V_{HS}}{V_{HS}^2} \frac{dT - TdV_{HS}}{V_{HS}} \quad (81)$$

This can be rearranged to

$$dP = \frac{zMRT}{V_{HS}} \left(\frac{dT}{T} - \frac{dV_{HS}}{V_{HS}} \right) = P \left(\frac{dT}{T} - \frac{dV_{HS}}{V_{HS}} \right) \quad (82)$$

Upon expressing these differentials as small but finite perturbations about the original operating point, denoted here by a zero subscript (The zero subscript here refers simply to a given operating point, not the overall reference point for the compensation calculation, as used elsewhere in this report.)

$$\delta P = P_o \left(\frac{\delta T}{T_o} - \frac{\delta V_{HS}}{V_{HS_o}} \right) \quad (83)$$

For the sake of algebraic simplicity, consider the case where there are no changes in the volume of the test container (this effect is usually very small compared to the volume change in the brine/waste, as was demonstrated in the example in Section 9.1). Volume variation in the brine/waste has been considered to occur only from thermal expansion/contraction effects (see discussion in Section 6.1.2). Again, for algebraic simplicity, express the volume change in the brine/waste, dV_b , as in Eqn. (42), rather than as in Eqn. (43). With these simplifications,

$$\delta V = - \delta V_l = \beta V_{l_o} \delta T \quad (84)$$

Substituting Eqn. (84) into Eqn. (83) and rearranging shows that the sensitivity of the pressure to variations in temperature will be

$$\delta P = P_0 \left(\frac{1}{T_o} + \frac{\beta}{V_{HS_o}/V_{l_o}} \right) \delta T \quad (85)$$

12.1 Pressure Sensitivity to Operating Pressure

Consider the situation where two experiments have identical ratios of headspace and liquid, i.e., the term V_{HS-o}/V_{l-o} is the same for both experiments (regardless of the test-container volume). With the same brine/waste (i.e., equal β) and operating at the same temperature, T_o , Eqn. (85) shows that the pressure perturbation is proportional to the operating pressure. An identical temperature perturbation, dT , in both experiments produces pressure perturbations that are proportionately more pronounced in the higher operating-pressure test container.

12.2 Pressure Sensitivity to Headspace/Waste Volume Ratio

Most investigations into gas-generation behavior monitor the experiment pressure to surmise the extent of gross gas generation. An objective of the GGE program was to identify the specific gases generated. Pressure measurements were intended only to provide backup information. Furthermore, the GGE program used actual TRU wastes immersed in brine with prototypic waste packing. Other investigations frequently overload the experiments with metals to artificially increase the quantity of gases generated over a specified time interval for a given brine/waste volume. This non-prototypicality produces measurable generated gas quantities rapidly, with correspondingly rapid pressure increases, even in relatively large headspace-gas volumes. On the other hand, the prototypic GGE program required relatively small headspace volumes to develop measurable generated-gas concentrations in the headspace.

Consider, again, Eqn. (85), but now from the viewpoint of two experiments with the same brine/waste, operating at the same temperature and pressure, but which have different ratios of headspace volume to brine/waste volume, V_{HS-o}/V_{l-o} . Once more, the actual volume of the test container is unimportant. Since all of the terms in Eqn. (85) are positive quantities, the experiment having the smaller headspace-to-brine/waste volume ratio will experience the greater pressure perturbation for a given temperature perturbation.

12.3 Comparison of the GGE to Other Gas-Generation Experiments

GGE test containers typically operated at approximately 14.824 MPa (2150 psia), about 146 standard atmospheres, and 30°C. The test containers were loaded to headspace-to-brine/waste volume ratios on the order of 0.1. The volumetric coefficient of thermal expansion in the brine/waste was found to be typically on the order of $0.38\text{E-}3 \text{ K}^{-1}$. Evaluating Eqn. (85) with these parameters shows that the GGE should anticipate a pressure sensitivity of

$$\frac{\delta P}{\delta T} = 14.824 \text{ MPa} \left[\frac{1}{303.15 \text{ K}} + \frac{0.38 \text{ E} - 3 \text{ K}^{-1}}{0.1} \right] = 105.49 \text{ kPa/C} \quad (15.3 \text{ psi/C})$$

The example in Section 9.1 showed that the sensitivity of the GGE experiments to temperature variation was, indeed, observed to have about this value.

Sections 12.1 and 12.2 showed that experiments conducted at pressures lower than those in the GGE program and/or those having larger ratios of headspace volume to brine/waste volume would experience smaller pressure perturbations. As an interesting comparison, Ref. 9 is an excellent report on the results of an investigation into gas-generation mechanisms conducted by Pacific Northwest National Laboratory on behalf of Sandia National Laboratory. Those experiments used the same Brine-A formulation as in GGE. The experiments were typically run at about 10 atm pressure, and with the same temperature specification of 30 +/- 5°C as in the GGE program. Headspace-to-brine/waste volume ratios, however, were approximately 0.37 (*ibid.*, Section 6.1.1). Under these conditions, and assuming comparable brine/waste thermal-expansion coefficients, Eqn. (85) shows that the pressure sensitivity in those experiments should be

$$\frac{\delta P}{\delta T} = 1.0135 \text{ MPa} \left[\frac{1}{303.15 \text{ K}} + \frac{0.38 \text{ E} - 3 \text{ K}^{-1}}{0.37} \right] = 4.413 \text{ kPa/C} \quad (0.64 \text{ psi/C})$$

This is far less than the 105.49 kPa/C (15.3 psi/C) found in the GGE, and accounts for the very smooth pressure measurements reported in Ref. 9.

13.0 Limitations of the Analyses

The methodology presented here is far from perfect. There are numerous limitations imposed on the reconstruction of the pressure data by shortcomings in the method of analysis and, in a few instances, by inaccuracies in the data. The list below identifies numerous potential pitfalls in both areas.

1. The experiment and the temperature and pressure behavior are transient, whereas the compensation methodology treats each data point as a steady-state condition. The entire pressure response is presumed to be well represented by a succession of steady state variations, not just point to adjacent point, but also between a point and the reference point.
2. The thermal expansion/contraction coefficients were based on the temperature-step data produced deliberately and with some degree of uncertainty. These were also generated at one point in time, after the experiments had been running for nearly three years. The value so found was then applied to the entire data set over the multi-year time frame. Any changes that may have occurred in this parameter over time would not have been known.
3. There were calibration corrections frequently made to both the RTD temperature sensors as well as to the pressure transducers. Although corrections were made, the

rate of degradation was not known. Degradation of these instruments was assumed to have occurred through a gradual and uniform process between consecutive calibration points.

4. The local temperature within the glovebox was estimated from some simple experiments under limited conditions. It is known that the local temperature is influenced somewhat by operation of the argon gas circulators, the number and location of the test-container heaters that are on at any one time, etc., but these secondary effects were not quantitatively explored.
5. Any leakage of headspace gas from the test containers would affect the true pressure data. The perfect containment of high-pressure gas at about 14.824 MPa (2150 psig) over periods of several years in a mechanically fastened container without the use of elastomer seals and subjected to thermal cycling is challenging.
6. At any one time there were perturbations to the system from calibrations, routine maintenance of equipment, equipment repairs and change out, equipment malfunctions (e.g., the MO-120 gas-purification unit), power outages, etc., all of which introduce some degree of upset to the system.
7. The test-container heaters were intended to control the test-container (RTD) temperature, but the feedback loop was sensing an auxiliary thermocouple mounted on the outside of the test container jacket, rather than the test-container RTD.
8. The off-line experimental measurement of β for brine was made at atmospheric pressure instead of at the high operating pressure. Published density data for water shows some slight effect of pressure.
9. There are a host of physical properties that are used in the methodology, particularly the thermal model, that may contain some error. For some properties, the brine was approximated as being water (e.g., the solubility treatment used parameters that pertain to gas diffusion in water).
10. The smearing of penetrations and other features in the head region to axisymmetrical geometry compromised the thermal models to some extent.
11. Assumptions had to be made for gap and contact conductances in the thermal models.
12. The role of solubility in determining the headspace-gas mass was estimated from a simplified model of the transport characteristics of gas diffusion in the liquid.
13. The experimental determination of the headspace volume may have introduced some error.
14. The physical dimensions used for transport surface areas were best estimates.

15. The idealized convection models used in the brine and in the headspace in the thermal models probably introduced some error.
16. The simplified one-dimensional thermal model and the constant-factor approach taken for handling two-dimensional effects in the test-container head region was known to be only a crude approximation.
17. There are angular non-uniformities in the heating (the heater bands covered only about 300 degrees of the test container circumference, whereas the thermal model is based on uniform circumferential conditions. The 60-degree gaps were not uniformly located on all the containers.
18. The dead bands in the heater controller cause lags in the temperature control.
19. Roundoff of temperature and pressure measurements to one decimal place were made by the data-acquisition system.
20. There were occasionally anomalous data recorded in the database.
21. There were some small discrepancies in the instrument-calibration records noted as to whether consistent terminology was used regarding how the instrument read relative to the standard during calibrations, and some incompleteness in the records was noted.
22. Generated gases originate as bubbles that may remain attached to the waste, or trapped and prevented from reaching the headspace. This does not affect the pressure response, but would allow the gases to be dissolved in the brine more readily (this would also make the headspace gas composition as determined from samples non-representative of the true composition).

Considering all of the many limitations listed above, the best criterion for evaluating the worth of the effort is the comparison of the compensated pressures at specific points to the measured data for the blank, control vessels, Test Containers No. 152 and 153. These were developed in Section 9.1 (Fig. 20 and Fig. 21). On that basis, the methodology appears to provide very acceptable results.

REFERENCES

1. L. Haar, J. S. Gallagher, and G. S. Kell, "*NBS/NRC Steam Tables - Thermodynamic and Transport Properties and Computer Programs for Vapor and Liquid States of Water in SI Units*," Hemisphere Publishing Corporation, Washington, D. C. (1984).
2. G. J. Van Wylen, "*Thermodynamics*," John Wiley & Sons, New York (1963).
3. D. R. Lide, editor, "*Handbook of Chemistry and Physics*," 74th ed., Chemical Rubber Co., CRC Press, Boca Raton (1993).
4. J. A. Dean, editor, "*Lange's Handbook of Chemistry*," 14th ed., McGraw-Hill, Inc, New York (1992).
5. N. Ernest Dorsey, editor, "*Properties of Ordinary Water Substance*," American Chemical Society, Book Dept., Reinhold Publishing Corp., New York (1940).
6. W. F. Linke, editor, "*Solubilities - Inorganic and Metal-Organic Compounds, K-Z; A Compilation of Solubility Data from the Periodic Literature*," 4th ed., **2**, American Chemical Society, Washington, D.C. (1965).
7. C. L. Yaws, et. al., "*Calculating Solubility and Henry's Law Constants for Gases in Water*," *Chem. Eng.* 106(6): (June 1999).
8. P. R. Hart to D. G. Cummings, Argonne National Laboratory-West, personal communication (August 18, 1995).
9. M. R. Telander and R. E. Westerman, "*Hydrogen Generation by Metal Corrosion in Simulated Waste Isolation Pilot Plant Environments*," Battelle Pacific Northwest Laboratory Report, SAND96-2538 (March 1997).
10. American Society for Metals, "*ASM Metals Reference Book*," **3**:155, Metals Park, OH (1993).
11. Y. Li and S. Gregory, "*Diffusion of Ions in Sea Water and in Deep Sea Sediments*," *Geochimica et Cosmochimica Acta*, **38**:703-714 (May 1974).
12. H. S. Carslaw and J. C. Jaeger, "*The Conduction of Heat in Solids*," 2nd Ed., Oxford Press, London, England (1959).
13. J. M. Coulson and J. F. Richardson, "*Chemical Engineering*," Revised 2nd Ed., **1**, Pergamon Press, Oxford England (1965).
14. E. R. G. Eckert and R. M. Drake, Jr., "*Analysis of Heat and Mass Transfer*," McGraw-Hill Book Company, New York (1972).

15. J. Barnes to F. S. Felisone, Bechtel BWXT Idaho Technologies, personal communication (1999).
16. Riley, editor "*Chemical Oceanography*," 2nd Ed., 4:338 (1975).

ACKNOWLEDGMENT

This work was part of an ANL-West effort supported by the DOE Carlsbad Field Office through SNL. Principal Investigator was Andrew Peterson, SNL. The funding support provided by Dave Duncan, former ANL-West GGE Project Manager and the continued encouragement by Carla Dwight, former ANL-West Waste Programs Manager, made the work possible and kept the study moving forward.

The assistance and support of several colleagues at ANL-West is gratefully acknowledged. Conversations with Joe Mitchell and Dan Cummings concerning the initial efforts to resolve this problem were very helpful and appreciated. Bryan Forsmann and Gary Schwartzenberger set up and conscientiously maintained the auxiliary experiment apparatus used for making the measurements of the thermal-expansion coefficients for the brine. Larry Foulkrod was very supportive and generous with his time whenever called upon to make numerous adjustments to the actual GGE experiment equipment needed to support this investigation.

APPENDIX A

Gas-Solubility Variation

The formulation used in the compensation methodology considered the effects of gas solubility in the brine. Solubility parameters were taken from the literature to specify the quantity of gas dissolved in the brine under given temperature and pressure conditions. These were equilibrium values. It is instructive to examine the rate of transport to assess the extent to which equilibrium values are relevant.

A1. Diffusion Model

Consider first a limiting case where all transport of gas through the brine is by diffusion only. This is an easily obtained solution that, although unrealistic, provides some feel for the problem. The 361-mm-deep body of brine liquid is in contact with headspace gas at some given pressure. The concentration of gas throughout the liquid is initially uniform at the equilibrium value, C_0 , that corresponds to the initial conditions. At time zero conditions change, causing the dissolved-gas concentration to seek a new equilibrium value, C_2 . In an infinitesimally thin layer at the surface, the gas concentration can be assumed to instantaneously achieve the value, C_2 , which could be found from Henry's Law, which states that, at constant temperature, the mole fraction of a dissolved gas is proportional to the partial pressure of that gas above the liquid surface. The physical arrangement and the general behavior of the dissolved-gas concentration is shown in Fig. A1. The diffusion of gas through the brine is described by (Ref. 13)

Fig. A1. Diffusion Model for Headspace-Gas Solubility

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial y^2} \quad (\text{A1})$$

This equation is subject to the conditions that

$$\begin{aligned} C &= C_0 \text{ at } t = 0 \text{ for all values of } y \\ C &= C_2 \text{ at } y = 0 \text{ for all values of } t \\ C &\rightarrow C_2 \text{ as } t \rightarrow \infty \text{ for all values of } y \end{aligned} \quad (\text{A2})$$

A non-dimensional, normalized gas concentration in the liquid can be defined as

$$\theta = \frac{C - C_0}{C_2 - C_0} \quad (\text{A3})$$

In terms of this variable, the boundary conditions become

$$\begin{aligned} \theta &= 0 & \text{at } t = 0 \text{ for all } y \\ \theta &= 1 & \text{at } y = 0 \text{ for all } t \\ \theta &\rightarrow 1 & \text{at } t \rightarrow \infty \text{ for all } y \end{aligned} \quad (\text{A4})$$

The analogous heat-transfer problem is one of conduction in a slab of given thickness, initially at uniform temperature and starting at time zero one face is held constant at a new temperature, with the opposite face perfectly insulated. The solution to this classic problem is given in Ref. 12 and an adaptation is plotted in Fig. A2. Since the heat-diffusion equation is analogous to the mass-diffusion equation, the solution applies as well to the present problem. The approach to the new equilibrium value is asymptotic, but the figure shows that about 98% of the eventual change has occurred when the quantity Dt/l^2 reaches the value of about 1.5. The diffusion coefficient for nitrogen diffusing through *water* at room temperature is about $1.64\text{e-}9 \text{ m}^2/\text{s}$ (Ref. 13). So the time required to reach 98% of the new equilibrium value is

$$t = 1.5 \frac{l^2}{D} = 1.5 \frac{(0.361\text{m})^2}{1.64\text{E-}9\text{m}^2/\text{s}} = 1.192\text{E} + 8 \text{ s}$$

Fig. A2. Solution to the Pure Diffusion Model

That is, about 3.8 years! Even for the dissolved-gas concentration to reach, on average, only 50% of the new equilibrium concentration the solution shows that a value for Dt/l^2 of about 0.25 is required, i.e., approximately 7.5 months.

A2. Diffusion/Convection Model

Transport in the GGE test containers will not be simply by diffusion, but, instead, will be augmented by the thermally induced natural convection. This will enhance the rate of movement of dissolved gas through the brine compared to that in the pure diffusion analysis presented above. Therefore, before gas solubility can be dismissed, the transport of gas via convection in the brine needs to be assessed. This will be a far more realistic solution than was presented in Section A1.

This can be estimated as follows. The discussion of natural convection within the brine/waste (Section 8.1) can be interpreted as a core of well-mixed fluid capped above and below by a thin layer of liquid across which all heat transport is by conduction. The same model can be applied to the transport of gas into, out of, and within the brine, since thermal buoyancy generates the natural convection. These same convective currents will be responsible for transport of the gas dissolved in the brine. Therefore, the “conduction layer” that pertains to the thermal problem will apply as well to the mass-transport analysis. This conduction-layer “thickness” can be estimated from the thermal model depicted in Fig. A3, which is similar to Fig. 15. The surface is at

temperature T_2 , and the concentration of gas, in moles per unit volume, dissolved just at the surface of the brine is C_2 . The heat-transfer rate is augmented by the natural convection. This can be represented by the use of an “effective” value for the thermal-conductivity coefficient, k_{eff} , defined such that the rate of heat transfer across the brine is

$$q = \frac{k_{eff}}{l}(T_2 - T_3) \quad (A5)$$

Fig. A3. Heat-Conduction and Convection Model for Determining the Temperature

The coefficient of thermal conductivity for molecular transport is k . Clearly, k_{eff}/k is greater than or equal to unity, where unity is the value if there were only molecular conduction throughout the brine.

The heat is presumed to be transferred across the “conduction” depth L to the bulk fluid at temperature T_m (the “mean” temperature) only by molecular conduction. Therefore, if the heat capacity of the thin “conduction layer” is ignored, the heat flux at the brine surface, denoted by the zero subscript, is

$$q_0 = -k \frac{dT}{dy} \Big|_{y=0} \approx -k \frac{\Delta T}{\Delta y} \Big|_{y=0} = -k \frac{(T_m - T_2)}{L} \quad (A6)$$

Since the heat fluxes in Equations (A5) and (A6) must be equal, the “conduction thickness” can be found by equating these expressions, yielding

$$L = \frac{1}{2} \frac{l}{[k_{eff}/k]} \quad (A7)$$

The ratio k_{eff}/k from experimental data in the literature is shown in Fig. A4 a function of the Ralieg number (14), itself a product of the Grashoff and Prandtl numbers:

$$Ra = Gr \cdot Pr = \frac{g\beta\Delta T l^3}{\nu^2} \cdot \frac{\nu}{\kappa} \quad (A8)$$

Equivalent heat conductivity for free convection through fluid layers.
From H. Kraussold, *Forsch. Gebiete Ingenieurw.*, 5:83 (1934).]

Fig. A4. Enhancement to the Thermal Conductivity to Account for Natural Convection

The Grashoff number is a ratio of buoyancy-induced forces (natural convection) to the viscous forces, and the Prandtl number relates viscous and thermal inertial terms. Therefore, the product of these two numbers is indicative of how natural convection of heat compares to the molecular conduction of heat. Taking the viscosity and thermal diffusivity of the brine to be those of water, with the test-container brine depth of about 361 mm gives a Ralieg number of about 1.4×10^9 . Extrapolating Fig. A4 suggests the ratio of effective thermal conductivity to the molecular value is

$$\frac{k_{eff}}{k} \approx 28.2$$

$$\dot{N}_g(t) = -D \frac{dC}{dy} \Big|_{y=0} \quad (\text{A9})$$

Referring to Fig. A5 (and, as was done with the thermal model, neglecting the gas quantity dissolved within the thin “diffusion layer”), this can be written as

$$\dot{N}_g(t) = -D \frac{[C_m(t) - C_2]}{L} \quad (\text{A10})$$

Now a balance is made on the quantity of gas dissolved. Over an infinitesimally short time interval, dt , the increase in the quantity of gas dissolved in the brine (moles) equals the quantity of gas (moles) transported into the brine during this time interval, or

$$dN_g = \dot{N}_g(t)A_c dt \quad (\text{A11})$$

In Eqn. (A11) A_c is the brine surface area (the cross-sectional area of the test container). This gives a differential equation that describes the quantity of gas dissolved over time. This equation can be recast in terms of the mass fraction of gas in solution, if desired. However, the solution process is *much* simpler when solved in terms of the dissolved-gas molar concentration, which is related to the number of moles of dissolved gas by

$$C_m = \frac{N_g}{V_l} \quad (\text{A12})$$

Differentiating Eqn. (A12),

$$dN_g = V_l dC_m \quad (\text{A13})$$

Substituting Equations (A10) and (A13) into Eqn. (A11) gives

$$dC_m = -\frac{2Dk_{eff}A_c}{l k V_l}(C_m - C_2)dt \quad (\text{A14})$$

The quotient A_c/V_l is just the inverse of the brine/waste depth, l . Rearranging gives

$$d(C_m - C_2) = -\frac{2D}{l^2} \frac{k_{eff}}{k}(C_m - C_2)dt \quad (\text{A15})$$

This can be directly integrated, with the result

$$\log_e\left(\frac{C_m - C_2}{C_0 - C_2}\right) = -\frac{2D}{l^2}\left(\frac{k_{eff}}{k}\right)t \quad (\text{A16})$$

As before, a non-dimensional, normalized dissolved gas concentration is defined, but in this case it refers to the mean, or bulk, concentration, which is a function only of time and not of depth. This is written as q_m , such that

$$\theta_m = \frac{C_m - C_0}{C_2 - C_0} \quad (\text{A17})$$

Clearly as time increases from zero to infinity, q_m varies as

$$0 \leq \theta_m \leq 1 \quad (\text{A18})$$

The solution, Eqn. (A16), can then be rewritten as

$$\theta_m = 1 - e^{-\frac{2D(k_{eff})}{l^2}t} \quad (\text{A19})$$

Finally, this can be rearranged to give the time explicitly as a function of the normalized concentration:

$$t = -\frac{l^2}{2D\left(\frac{k_{eff}}{k}\right)} \log_e (1 - \theta_m) \quad (\text{A20})$$

The same example as before, Section A1, is now evaluated. The multiplier term in Eqn. (A20) gives $1.41e+6$ s. For a mean, normalized gas-concentration change of 98%, the log term is found to be -3.91. Therefore, the time required for the bulk gas concentration in the brine to achieve 98% of the ultimate new equilibrium gas concentration is

$$t = -1.41e+6 \text{ s}(-3.91) = 5.51e+6 \text{ s} \approx 64 \text{ days}$$

Similarly, for the dissolved-gas concentration to change to only 50% of the ultimate new equilibrium value requires over 11 days.

As expected, the time durations found with this analysis that includes a more realistic gas-transport mechanism are much shorter than were calculated on the basis of purely diffusive transport throughout the entire brine volume, even with the relatively meager natural convection generated by temperature differences of only a few degrees Celsius. Nevertheless, for nitrogen gas, at least, the rate of change in the quantity of dissolved gas, and therefore the effect on headspace gas mass, due to gas solubility variation can be concluded to be so slow that the impact on the methodology addressed in this report is insignificant. Long before the bulk dissolved gas concentration approaches the new equilibrium value, the conditions will have changed yet again.

These results are based on the diffusion of gases in pure water. Diffusion coefficients of gases decrease somewhat with increasing salinity as shown in Ref. 11 using viscosities calculated per Ref. 16. Therefore, it should be expected that changes in the quantity of gas dissolved in brine would occur even more slowly than discussed here.

The diffusion coefficient for hydrogen gas in water is 1.6 times that for nitrogen in water (5). This shortens the times computed in this section proportionately, Eqn. (A20), but since the predominant gas is nitrogen, the conclusions with regard to solubility affecting the headspace-gas mass remain valid.

APPENDIX B

Thermal Expansion Experiments

A special experimental apparatus was set up to determine the thermal expansion coefficient of brine in order to validate the data and the analysis methodology. These experiments are described in this appendix.

Figure B1 depicts the experiment. A closed container was immersed in a circulating, temperature-controlled bath. The internal volume of the container was calculated from careful dimensional measurements. The container was filled with the liquid under investigation (pure distilled water or brine), the heater was energized and the system was allowed to come to a steady state. The liquid level was adjusted so that the level just indicated on a graduated pipette mounted on the container. Careful temperature measurements were made in several places to enable the best estimate of the mean liquid temperature to be obtained.

Fig. B1. Experiment Configuration for Determination of the Volumetric, Thermal-Expansion Coefficients for Pure Water and Brine

The temperature setting on the heater was then adjusted upward. Following the obtainment of new steady conditions the temperatures were recorded along with the new reading on the graduated pipette. The volume change of the test container itself as a result of the new temperature was estimated. Since the quantity of liquid within the container and the pipette was

constant, an expansion coefficient could be calculated from the pipette reading and the temperature map. Photographs of the experimental apparatus are shown in Fig. B2—Fig. B4.

Fig. B2. Experiment Apparatus for Determination of the Volumetric, Thermal-Expansion Coefficient

Fig. B3. Test Vessel for the Thermal-Expansion Measurements

Fig. B4. Top View of the Test Vessel in its Water Bath

The apparatus was first used to check data on pure water against expansion coefficients that could be deduced from the saturated-water data in the steam tables (1). It was during these experiments that the strong influence of residual bubbles in the liquid was noted. The test vessel lid was made of a transparent material that allowed bubbles to be observed. To overcome these problems, the container was drained, very thoroughly cleaned and refilled very slowly. The container was also tilted slightly to ensure that any gas bubbles had an easy path to escape from the pipette that was mounted on the vessel lid as close to the edge as possible. After filling, the apparatus was allowed to sit for several days to release all of the bubbles. Figure B5 shows the data for water plotted against values deduced from the steam tables for temperatures within the range of interest to GGE and for both local atmospheric pressure, 85 kPa (12.33 psia), and an elevated pressure of 14.8 MPa (2147 psia), typical of the GGE pressures. The experimental apparatus could only be operated at atmospheric pressure. The agreement of the experimental data to that deduced from published information was found to be excellent. This provided the confidence that high-quality measurements could be made on pure brine with this apparatus.

Brine identical to that used in the GGE experiments was loaded into the test apparatus. A series of data points were generated at different temperatures. The results are shown in Figure B6.

Fig. B5. Measured Volumetric Coefficients of Thermal-Expansion for Pure Water

Fig. B6. Measured Volumetric Coefficients of Thermal-Expansion for Brine A

An early intent had been to repeat these experiments with measurements on brine/waste mixtures. The difficulties encountered with bubbles during the initial measurements with water indicated quite clearly that any attempts to make measurements on brine/waste would be subject to large errors.

Data-reduction sheets for one data point shown in each of Fig. B5 and Fig. B6 are provided at the end of this appendix.

ATTACHMENT TO APPENDIX B

Sheet 1 of 2

EXPERIMENTAL-MEASUREMENT DATA REDUCTION

Waste/Brine: Pure Water

	mo-day- yr	hr:min
Date/Time of Initial Data:	<u>10 - 07 - 98</u>	<u>11 : 32</u>
Date/Time of New Data:	<u>10 - 07 - 98</u>	<u>14 : 30</u>

1. Waste/Brine Temperature

Spatial Average

$$\begin{aligned}
 T_{1-0} &= 0.5 * [T_{1-upper} + T_{1-lower}]_0 = 0.5 * [\underline{28.0} + \underline{27.65}] = \underline{27.825}C \\
 T_1 &= 0.5 * [T_{1-upper} + T_{1-lower}] = 0.5 * [\underline{34.0} + \underline{33.45}] = \underline{33.725}C \\
 \Delta T_1 &= T_1 - T_{1-0} = \underline{33.725} - \underline{27.825} = \underline{5.90} C
 \end{aligned}$$

Change-Averaged Temperature

$$T_{1-change\ ave} = 0.5 * [T_{1-0} + T_1] = 0.5 * [\underline{27.825} + \underline{33.725}] = \underline{30.775}C$$

2. Bath Temperature - Ave.

$$\begin{aligned}
 T_{b-0} &= 0.5 * [T_{b-upper} + T_{b-lower}]_0 = 0.5 * [\underline{27.75} + \underline{27.95}] = \underline{27.85}C \\
 T_b &= 0.5 * [T_{b-upper} + T_{b-lower}] = 0.5 * [\underline{33.9} + \underline{34.05}] = \underline{33.975}C
 \end{aligned}$$

3. Container Temperature - Ave.

$$\begin{aligned}
 T_{c-0} &= 0.5 * [T_{b-0} + T_{1-0}] = 0.5 * [\underline{27.85} + \underline{27.825}] = \underline{27.838}C \\
 T_c &= 0.5 * [T_b + T_1] = 0.5 * [\underline{33.975} + \underline{33.725}] = \underline{33.85}C
 \end{aligned}$$

4. Container Ave. Temperature Change

$$\Delta T_c = T_c - T_{c-0} = \underline{33.85} - \underline{27.838} = \underline{6.01} C$$

5. Container Volume Change

$$\begin{aligned}
 \Delta V_c &= 3\alpha V_{c-0} \Delta T_c = 3 * 17.3e-6\ 1/C * 8944\ ml * \underline{6.01} C \\
 &= \underline{2.79} ml
 \end{aligned}$$

6. Pipette Volume Change

$$\begin{aligned}
 \Delta V_p &= V_p - V_{p-0} = (V_{p-tare} + 50.0 - V_{p-reading}) - \\
 &\quad (V_{p-tare} + 50.0 - V_{p-reading})_0 \\
 &= [5.2 + 50.0 - \underline{32.3}] - [5.2 + 50.0 - \underline{46.0}] ml \\
 &= \underline{13.70} ml
 \end{aligned}$$

7. Waste/Brine Volume Change

$$\Delta V_1 = \Delta V_c + \Delta V_p = \underline{2.79} + \underline{13.70} \text{ ml} = \underline{16.49} \text{ ml}$$

8. Waste/Brine Volume

$$\begin{aligned} V_{1-0} &= V_{c-0} + V_{p-0} = V_{c-0} + (V_{p\text{-tare}} + 50.0 - V_{p\text{-reading}})_0 \\ &= 8944 + 5.2 + (50.0 - \underline{46.0}) = \underline{8953.2} \text{ ml} \\ V_1 &= V_{1-0} + \Delta V_1 = \underline{8953.2} + \underline{16.49} = \underline{8969.7} \text{ ml} \end{aligned}$$

9. Expansion Coefficient at the change-averaged waste/brine temperature, $T_{1\text{-change ave}} = \underline{30.775} \text{ }^\circ\text{C}$:

$$\begin{aligned} \beta &= \ln (V_1/V_{1-0}) / \Delta T_1 \\ &= \ln (\underline{8969.7} / \underline{8953.2}) / \underline{5.90} \text{ }^\circ\text{C} \\ &= \underline{3.12 \times 10^{-4}} \text{ } 1/^\circ\text{C} \end{aligned}$$

EXPERIMENTAL-MEASUREMENT DATA REDUCTION

Waste/Brine: Brine-A

	mo-day- yr	hr:min
Date/Time of Initial Data:	<u>10 - 14 - 98</u>	<u>08 : 22</u>
Date/Time of New Data:	<u>10 - 14 - 98</u>	<u>11 : 35</u>

1. Waste/Brine Temperature

Spatial Average

$$\begin{aligned}
 T_{1-0} &= 0.5 * [T_{1\text{-upper}} + T_{1\text{-lower}}]_0 = 0.5 * [\underline{30.1} + \underline{30.0}] = \underline{30.05} \text{ C} \\
 T_1 &= 0.5 * [T_{1\text{-upper}} + T_{1\text{-lower}}] = 0.5 * [\underline{37.35} + \underline{37.1}] = \underline{37.225} \text{ C} \\
 \Delta T_1 &= T_1 - T_{1-0} = \underline{37.225} - \underline{30.05} = \underline{7.175} \text{ C}
 \end{aligned}$$

Change-Averaged Temperature

$$T_{1\text{-change ave}} = 0.5 * [T_{1-0} + T_1] = 0.5 * [\underline{30.05} + \underline{37.225}] = \underline{33.638} \text{ C}$$

2. Bath Temperature - Ave.

$$\begin{aligned}
 T_{b-0} &= 0.5 * [T_{b\text{-upper}} + T_{b\text{-lower}}]_0 = 0.5 * [\underline{30.3} + \underline{30.05}] = \underline{30.175} \text{ C} \\
 T_b &= 0.5 * [T_{b\text{-upper}} + T_{b\text{-lower}}] = 0.5 * [\underline{37.4} + \underline{37.4}] = \underline{37.4} \text{ C}
 \end{aligned}$$

3. Container Temperature - Ave.

$$\begin{aligned}
 T_{c-0} &= 0.5 * [T_{b-0} + T_{1-0}] = 0.5 * [\underline{30.175} + \underline{30.05}] = \underline{30.113} \text{ C} \\
 T_c &= 0.5 * [T_b + T_1] = 0.5 * [\underline{37.4} + \underline{37.225}] = \underline{37.313} \text{ C}
 \end{aligned}$$

4. Container Ave. Temperature Change

$$\Delta T_c = T_c - T_{c-0} = \underline{37.313} - \underline{30.113} = \underline{7.20} \text{ C}$$

5. Container Volume Change

$$\begin{aligned}
 \Delta V_c &= 3\alpha V_{c-0} \Delta T_c = 3 * 17.3\text{e-}6 \text{ 1/C} * 8944 \text{ ml} * \underline{7.20} \text{ C} \\
 &= \underline{3.34} \text{ ml}
 \end{aligned}$$

6. Pipette Volume Change

$$\begin{aligned}
 \Delta V_p &= V_p - V_{p-0} = (V_{p\text{-tare}} + 50.0 - V_{p\text{-reading}}) - \\
 &\quad (V_{p\text{-tare}} + 50.0 - V_{p\text{-reading}})_0 \\
 &= [5.2 + 50.0 - \underline{23.8}] - [5.2 + 50.0 - \underline{44.9}] \text{ ml} \\
 &= \underline{21.10} \text{ ml}
 \end{aligned}$$

7. Waste/Brine Volume Change

$$\Delta V_1 = \Delta V_c + \Delta V_p = \underline{3.34} + \underline{21.10} \text{ ml} = \underline{24.44} \text{ ml}$$

8. Waste/Brine Volume

$$\begin{aligned} V_{1-0} &= V_{c-0} + V_{p-0} = V_{c-0} + (V_{p\text{-tare}} + 50.0 - V_{p\text{-reading}})_0 \\ &= 8944 + 5.2 + (50.0 - \underline{44.9}) = \underline{8954.3} \text{ ml} \\ V_1 &= V_{1-0} + \Delta V_1 = \underline{8954.3} + \underline{24.44} = \underline{8978.7} \text{ ml} \end{aligned}$$

9. Expansion Coefficient at the change-averaged waste/brine temperature, $T_{1\text{-change ave}} = \underline{33.638} \text{ C}$:

$$\begin{aligned} \beta &= \ln (V_1/V_{1-0}) / \Delta T_1 \\ &= \ln (\underline{8978.7} / \underline{8954.3}) / \underline{7.175} \text{ C} \\ &= \underline{3.799(6)} \times 10^{-4} \text{ 1/C} \end{aligned}$$

APPENDIX C

Local Glovebox Temperature Determination

An attempt was made to account for the amount by which the local temperature within the glovebox exceeded the measurement recorded by the “glovebox RTD”. The difference between the actual local temperature in the vicinity of the test vessel head and the temperature measured by the glovebox RTD was termed the “excess” temperature.

C1. Temperature Mapping

The glovebox RTD was mounted in its normal position underneath the subfloor and against the wall of the glovebox. An auxiliary RTD was moved around the glovebox to create a map of the temperatures for comparison to that measured by the fixed RTD. Attached to this appendix is a summary communication of the mapping effort and the results found.

Another session successively placed the auxiliary RTD in the head region between test containers. The temperature measurements from this RTD were compared to those measured by the fixed glovebox RTD. The variation in these measurements throughout the glovebox were modest, with an approximately constant deviation from the temperature measured by the glovebox RTD.

C2. Excess-Temperature Algorithm

The local temperature is actually subject to various influences: number and location of test vessel heaters that may be energized at any time; argon-gas circulation and oxygen-removal equipment function, lighting heat load, etc. The variability of these influences was not investigated. Instead, the excess temperature was assumed to be simply a function of the glovebox temperature measurements.

A number of data points from the exercises described above were plotted against the glovebox temperature measurement and a 2nd-order polynomial fit was made to the data using a Microsoft Excel plotting function. Since the experiments found that the excess temperature approaches a constant value of 2-3°C as the glovebox temperature approaches the test-containers’ set-point value of 30°C, a linear fit was deemed inappropriate. The basis for selecting a 2nd-order polynomial fit was that the excess temperature should be a monotonic function of the glovebox temperature (higher-order polynomials would not necessarily be monotonic).

The data points and the curve-fit are shown in Fig. C1. The equation for this curve is

$$\Delta T_{ex} = 0.0215T_{GB}^2 - 1.2975T_{GB} + 21.503 \quad (C1)$$

This algorithm was applied consistently to all of the archived data.

Fig. C1. Estimate of Local Test Container Temperature Excess

ATTACHMENT TO APPENDIX C

Observations from An Impromptu Experiment - GGE

FSF 9-98

Larry Foulkrod and Frank Felicione performed an impromptu, informal experiment to determine if the "glovebox temperature" measurement was influenced by the location where it was measured. This is described below. The experiment was done on 09-03-98, between ~10:30 to 11:30.

The system was running steadily, no gross circulation in the box, and there was no activity in the area. All measurements were made using the RTD's that were in place and connected to the DAS.

Temperature - Measurement Positions:

South Elevation

East Elevation

Initial Temperatures:	A	25.3 C
	B	26.6
	C	26.8
	D	-
	E	~30.5 (ave., actual TC's varied from 30.3 - 30.8 C)
	F	-
	G	-

Position A is the "glovebox temperature" measurement. There are RTD's lying on the false floor (rather haphazardly) at positions B and C.

Experiment :

- 1) Remove RTD from position A (next to wall) and place near position B/C (on the false floor, within a few inches of each other). Result: 26.5 C after ~10 min and apparently steady.
- 2) Move this same RTD to position F (~ same depth below the false floor as position A, but away from the wall). Result: 26.5 C (ie., no change from position B/C).
- 3) Move this same RTD to position G. Result: >27.2 C (ie., not quite equilibrated after ~5 min).
- 4) Move RTD from position C to position D (hanging from hoist chain). Result: 28.1 C

Conclusions :

- 1) There are temperature gradients within the glovebox. These very likely result from the heat input to the TC heaters, although the ZPPR cell temperature may also have temperature gradients within.
- 2) Temperature measurements at position A are affected by the wall temperature and are not a good indicator of the temperature just above the TC's. Positions B/C provide a better indication, but the temperature measured here is probably somewhat cooler than that at the same elevation (just above the false floor) but in the region where the heated TC's are located [the lead length on the RTD would not allow it to be repositioned to this area during this experiment].

- 3) The result is that there is no historical record of the "glovebox temperature" that is representative of the temperature in the vicinity of the upper part of the TC's. These temperatures will have to be estimated on the basis of archived data at positions A, B, & C. [Larry Fulkrod has cautioned that the RTD's at positions B/C may have not always been at these same positions!].

This will impact our ability to unravel the historical pressure variation to some extent.

10-15-98

~09:30

Larry Foulkrod moved RTD No. 15 and 16 to positions more representative of the GB environment surrounding the TC's.

Both RTD's were moved to a lateral position very near the center of the heated TC region. No. 15 was placed about 6 in above the false floor, i.e., at an elevation equal to that at the top of the TC's. No. 16 was placed ~ 2 in below the false floor. These are positioned along the GB centerline and between TC positions 05 & 07.

In their original positions (positions B & C on the figure, p.1) these both read 26.8 C. In their new positions they show

RTD No. 15 28.0 C

RTD No. 16 27.9 C

At the same time the "GB Temperature" (position A, p.1) read 25.5 C. The TC RTD's varied from 29.9 to 30.6 C.

APPENDIX D

Computer Application Program

The entire pressure-compensation methodology was formulated as an adjustment to the measured pressure, where all of the influences other than gas generation were methodically stripped out of the results. The analysis was programmed for computer application in FORTRAN. The final computer program, the result of evolutionary improvements, is titled *GGE7b1*.

D1. Program Input

The program may be applied to discrete data points entered manually or to a very large number of data points normally generated as an input listing from another software package. The former is useful for checkout or other special purposes; the latter “streaming-data-input” approach was used to facilitate input of the 26,000-plus data points for each test container that generated the results shown in Section 11.1.

Attachment 1 to this appendix is a listing of the input files that contain the unique information required to analyze each test container. These *set-up* files are all unformatted text (ASCII) file types, and are labeled

SETxxx.TXT

The *xxx* is the identification number of the test container, e.g., *SET160.TXT* pertains to TC-160, making each file unique to the corresponding test container. Each *SETxxx.TXT* file contains all of the set-up information required to analyze the given test-container data. This includes geometry, sampling data, RTD and PXD calibration data, the temperature-step data for calculating β_H and β_L , and miscellaneous physical properties.

A second group of files for the voluminous streaming data input carry the labels

STRxxx.TXT

Again, the *xxx* refers to a test-container identification number. The *STRxxx.TXT* files are unformatted text files that contain the full data set (test container and glovebox RTD data and pressure data, along with some specific parameters such as local glovebox temperature excess over the measurement) for each test container for use with the streaming-input option. The *STRxxx.TXT* files also contain indicators of duplicate or “dropped” data (zeros). A parameter, ISTRM, in the *SETxxx.TXT* file triggers whether the selected data points provided in the *SETxxx.TXT* file are used, or whether the streaming-input data file is to be read to supply this information.

Data from the data-acquisition system were transferred to a Microsoft EXCEL-97 spreadsheet program. Logic was programmed into these spreadsheet files to remove duplicated or “dropped” data (zeros) from the raw data-point sequence numbers in the file, resulting in a “valid” sequence numbering for the data. The spreadsheet also calculated the local glovebox temperature

algorithm (Appendix C). Unformatted text files, *STRxxx.TXT*, were then created from these spreadsheet files. A procedure for generating the *STRxxx.TXT* files is Attachment 2 to this appendix. These files are approximately 1.7 Mbytes for each test container, and consist of approximately 26,000 lines of printed data. A CD-ROM disk containing the 14 files for the GGE test containers has been placed in the GGE Project Files.

D2. Specification of the Test Container to be Analyzed

The selection of the actual test container to be analyzed by the application program is made by copying the selected *SETxxx.TXT* and *STRxxx.TXT* files, respectively, to the two identical-content files that are actually read by the *GGE7b1* application program:

GGESET.TXT
GGESTR.TXT

For example, to apply the data-adjustment methodology to data from test container No. 166, the file *SET166.TXT* needs to be copied to *GGESET.TXT* and (if the *streaming-data* option is to be used) the file *STR166.TXT* needs to be copied to *GGESTR.TXT*. The currently specified subdirectories for *GGESET.TXT* and *GGESTR.TXT* files are specified in two *OPEN* statements at the beginning of the application program.

D3. Program Output

Execution of the applications program results in the generation of two output files. The first, *GGE.OUT*, is an unformatted text file that contains virtually all of the intermediate results, mirrors the input, etc. This file is useful for checking intermediate calculations by the program, but becomes an extremely large file when many thousands of data points are analyzed. The second output file, *GGESUM.OUT*, is a summary unformatted text file that contains the raw pressure measurement and the adjusted pressure, but, to keep its size reasonable, virtually no intermediate calculations. This file is used for plotting the results, and was the origin of the plots shown in Section 11.1 in this report. The specific sub-directory paths for *GGE.OUT* and *GGESUM.OUT* files are specified in the *OPEN* statements at the beginning of the applications program, and these could easily be changed to whatever path is desired.

D4. Program Map and Listing

The programming for the complete methodology, including the one-dimensional thermal model, was developed specifically for this application. A top-level map that describes the logic flow through the programs is provided in Attachment 3 to this appendix. The listing of the FORTRAN source program, *GGE7b1*, is Attachment 4 to this appendix.

D5. Execution of the Program

The program was compiled and executed on Ryan-McFarland Corporation's RM/FORTRAN, Version 02.45.02, with program linking via Phoenix Software Associates Ltd. PLINK86 linker program. The program was run on an Intel Pentium II processor, operating at 233 MHZ.

Execution of the approximately 26,000 data points for each test container required approximately 2.25 minutes.

D6. Results Plots

The plots of the temperature, pressure, and mole fraction of generated gases were produced with the Microsoft EXCEL-97 spreadsheet program. The output *GGESUM.OUT* files were read into an EXCEL spreadsheet and plotted using the standard EXCEL plotting features.

ATTACHMENT 1 TO APPENDIX D

SET xxx. TXT Files Listings

The following pages contain the setup parameters for use in *Program GGE7b1* (SETxxx.txt files) in the following order:

Filename	Test Container ¹	No. of Sheets
SET151.txt	TC-151	(3 sheets)
SET152.txt	TC-152	(3 sheets)
SET153.txt	TC-153	(3 sheets)
SET160.txt	TC-160	(3 sheets)
SET161.txt	TC-161	(3 sheets)
SET161e.txt	TC-161e	(3 sheets)
SET162.txt	TC-162	(3 sheets)
SET163.txt	TC-163	(3 sheets)
SET164.txt	TC-164	(3 sheets)
SET165.txt	TC-165	(3 sheets)
SET166.txt	TC-166	(3 sheets)
SET167.txt	TC-167	(3 sheets)
SET168.txt	TC-168	(3 sheets)
SET169.txt	TC-169	(3 sheets)
SET170.txt	TC-170	(3 sheets)

1. SET161e.txt is the same as SET161.txt, but uses empirical, trial calibration factors for the brine/waste RTD (see discussion in Section 11.2.1).

ATTACHMENT 1 OF APPENDIX D

TC-151 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17	36.	0.059454
18	37.	0.062795
19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PRESS-XDUCER CALIBRATIONS: NCALT,NCALP
8 6

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	0	0.	0.
07-15-96:??	1080	0.	0.
01-13-97:??	5322	0.	0.1
07-09-97:??	9382	0.	0.1
11-21-97:??	11856	0.	0.
05-21-98:??	16852	0.	0.
11-23-98:??	21208	0.	0.
05-24-99:??	25371	0.	0.

PRESSURE-XDUCER CALIBRATION INFO: [DATE:HR],PT NO.,COMP.,RESIDP

05-24-96:??	2	0.	0.
11-14-96:??	3936	0.	0.
05-14-97:??	8065	0.	0.
12-02-97:??	12844	0.	0.
06-02-98:??	17134	0.	0.
12-07-98:??	21533	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP

10001	2170.1	31.0	29.3	1.94
-------	--------	------	------	------

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI

50	0.17	0.19
----	------	------

BRINE MASS AND MOLECULAR WEIGHT: AMB [G],WTMOLB [G/GMOLE]
7708. 18.5

UNIVERSAL GAS CONSTANT: RU [PSI*ML/GMOLE/K],ATM PRESS [PSIA]
1205.95 14.696

SOL GAS INFO: VOL FRACT[VFRG],MOL WT[WTMOLG],CONSTANTS A,B,C
1. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
4

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-02	143	2184.6	2175.2	30.35	21.5	3.51
-03	2699	2183.8	2174.2	30.55	21.6	2.07
-04	5407	2191.4	2182.0	31.3	29.65	1.93
-05	8017	2171.2	2161.8	30.6	28.0	2.02

PXD BACKFILL INFO: [NO.,PT.NO.],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	2	2128.3	2128.3	24.0	24.0	20.9	3.82
-02	3936	2178.3	2181.9	30.7	30.7	28.3	2.00
-03	8065	2161.8	2162.2	30.5	30.5	27.7	2.06
-04	12844	2155.0	2154.4	30.4	30.4	22.1	3.33
-05	17134	2153.9	2154.4	30.6	30.6	19.9	4.20
-06	21533	2154.6	2156.2	30.2	30.2	25.9	2.32

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS:NPTK,PK,TRTDK,TGBK,TEXK

23075	2142.3	29.6	20.0	4.15
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS:PB,TRTDB,TGBB,TEXB

23236	2078.5	25.0	20.8	3.82
-------	--------	------	------	------

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS:PK,TRTDK,TGBK,TEXK

22098	2155.0	30.2	26.1	2.28
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB,TRTDB,TGBB,TEXB

22122	2259.7	37.4	26.2	2.27
-------	--------	------	------	------

NUMBER OF DATA POINTS TO BE ADJUSTED, NDATA, AND INPUT KEY ISTRM

3 1

DATA-PT NO.,DATE&TIME,PRESS,RTD TEMP,GB TEMP,EXCESS TEMP

8001	05-11-97:18	2170.7	30.7	28.4	2.00
14001	01-20-98:16	2151.7	30.5	21.0	3.74
20001	10-02-98:09	2156.0	30.3	25.5	2.40

TC-152 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19 38. 0.066298
 20 39. 0.069969
 21 40. 0.073814
 TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
 7272. 11.3E-6
 GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
 0.
 NUMBER OF RTD & PRESS XDUCR CALIBRATIONS: NCALT,NCALP
 8 6
 RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR
 11-03-95:?? 1 0. -0.2
 07-15-96:?? 776 0. -0.2
 01-13-97:?? 5018 0. 0.
 07-09-97:?? 9079 0. 0.1
 11-21-97:?? 12294 0. 0.
 05-21-98:?? 16560 0. 0.1
 11-23-98:?? 20938 0. 0.
 05-24-99:?? 25099 0. 0.1
 PRESSURE XDUCER CALIBRATION INFO: [DATE:HR],PT NO, COMP, RESIDP
 06-06-96:?? 1 0. 0.
 12-05-96:?? 4126 0. 0.
 06-05-97:?? 8271 0. 0.
 12-02-97:?? 12550 0. 0.
 06-02-98:?? 16841 0. 0.
 12-07-98:?? 21259 0. 0.
 OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
 10001 2141.8 30.9 29.1 1.95
 HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
 50 0.17 0.19
 BRINE MASS AND MOLECULAR WEIGHT: AMB[G],WTMOLB[G/GMOLE]
 7894. 18.5
 UNIVERSAL GAS CONSTANT: RU[PSI*ML/GMOLE/K],STD ATM PRESS[PSIA]
 1205.95 14.696
 SOL GAS INFO: VOL FRACT[VFRG],MOL WT[WTMOLG],CONSTANTS A,B,C
 0. -67.3877 86.3213 24.7981
 SAMPLE VOLUME: VSAMPL
 3.05
 NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
 4
 GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX
 -02 91 2163.0 2153.1 30.0 21.45 3.58
 -03 2587 2153.8 2144.3 30.2 27.8 2.05
 -04 5243 2154.2 2144.7 30.7 28.6 1.97
 -05 7765 2139.6 2130.1 30.3 27.7 2.06
 PXD BACKFILL INFO: [NO.,PT NO.],PC1,PC2,TC1,TC2,TGBC,TGBEXC
 -01 1 2112.7 2112.7 22.7 22.7 21.9 3.40

-02	4126	2153.5	2155.7	30.8	30.8	28.6	1.98
-03	8271	2130.8	2131.6	30.3	30.3	27.6	2.07
-04	12550	2131.3	2131.0	30.9	30.9	22.1	3.33
-05	16841	2114.2	2114.2	30.0	29.9	19.6	4.33
-06	21259	2129.1	2129.1	30.6	30.6	25.9	2.32

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS: NPTK, PK, TRTDK, TGBK, TEXK

16058	2121.5	30.5	20.7	3.94
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

16206	2052.7	25.6	20.2	4.07
-------	--------	------	------	------

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS: PK, TRTDK, TGBK, TEXK

16058	2121.5	30.5	20.7	3.94
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

16077	2270.5	40.5	21.0	3.66
-------	--------	------	------	------

NUMBER OF DATA POINTS TO BE ADJUSTED AND INPUT KEY, ISTRM

3 1

DATA-PT NO., DATE&TIME, PRESS, RTD TEMP, GB TEMP, EXCESS TEMP

8001	05-25-97:01	2132.7	30.5	28.5	1.99
14001	02-01-98:19	2114.3	30.3	18.2	5.01
20001	10-14-98:10	2126.7	30.4	25.5	2.40

TC-153 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PRESS XDUCR CALIBRATIONS: NCALT,NCALP
8 6

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESIDT

11-03-95:??	0	0.	0.
07-15-96:14	597	0.	0.
01-13-97:??	4878	0.	0.
07-09-97:??	8976	0.	0.
11-21-97:??	12214	-0.1	0.
05-21-98:??	16539	0.	0.
11-23-98:??	20893	0.	0.
05-24-99:??	25058	0.	0.1

PRESSURE XDUCER CALIBRATION INFO: [DATE:HR],PT NO.,COMP,RESIDP

06-13-96:??	0	0.	0.
12-05-96:??	3982	0.	0.
06-05-97:??	8164	0.	0.
12-02-97:??	12477	0.	0.
06-02-98:??	16881	0.	0.
12-07-98:??	21220	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2154.2 31.0 29.3 1.94

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.15 0.19

BRINE MASS AND MOLECULAR WT: AMB [G],WTMOLB[G/GMOLE]
7868. 18.5

UNIVERSAL GAS CONSTANT:RU [PSI*ML/GMOLE/K],ATM PRESS [PSIA]
1205.95 14.696

SOL GAS INFO: VOL FRACT[VFRG],MOL WT[WTMOLG],CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
4

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-02	14	2190.1	2180.4	29.8	22.1	3.33
-03	2569	2171.7	2161.8	30.55	27.9	2.04
-04	5444	2165.0	2155.3	30.6	28.6	1.98
-05	8002	2155.7	2145.9	30.4	27.7	2.06

PXD BACKFILL INFO: [NO.,PT. NO.],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	1	2191.3	2191.3	29.5	29.5	22.1	3.33
-----	---	--------	--------	------	------	------	------

-02	3982	2166.8	2169.8	30.8	30.8	28.6	1.98
-03	8164	2144.1	2144.8	30.3	30.3	28.3	2.00
-04	12477	2125.9	2126.7	29.7	29.7	22.2	3.29
-05	16881	2122.2	2122.1	29.7	29.8	19.1	4.56
-06	21220	2138.1	2139.0	30.5	30.5	25.9	2.32

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS: NPTK, PK, TRTDK, TGBK, TEXK

16043	2119.0	29.6	20.6	3.90
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGGB, TEXB

16188	2064.8	25.7	20.4	3.98
-------	--------	------	------	------

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS: PK, TRTDK, TGBK, TEXK

16043	2119.0	29.6	20.6	3.90
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGGB, TEXB

16059	2270.4	39.8	20.9	3.78
-------	--------	------	------	------

NUMBER OF DATA POINTS TO BE ADJUSTED, NDATA, AND INPUT KEY, ISTRM

3 1

DATA-PT NO., DATE&TIME, PRESS, RTD TEMP, GB TEMP, EXCESS TEMP

8001	05-29-97:14	2156.2	30.6	27.9	2.04
14001	02-04-98:03	2110.8	29.3	18.2	5.01
20001	10-15-98:21	2136.9	30.5	25.6	2.38

TC-160 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PXD CALIBRATIONS: NCALT,NCALP
8 6

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESIDT

11-03-95:??	1	0.	0.
07-15-96:??	2306	0.	0.
01-13-97:??	6544	0.	-0.1
07-09-97:??	10609	0.	-0.1
11-21-97:??	13823	-0.3	0.
05-21-98:??	18111	0.	-0.1
11-23-98:??	22489	0.	0.
05-24-99:??	26678	0.	0.

PRESSURE XDUCER CALIBRATION: [DATE:HR],PT NO,COMP,RESIDP

08-13-96:10	2957	0.	0.
02-21-97:??	7428	0.	0.
08-21-97:??	11632	0.	0.
02-20-98:??	15981	0.	0.
08-19-98:??	20240	0.	0.
02-17-99:??	24409	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2128.0 31.2 28.6 1.98

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.17 0.19

BRINE MASS & MOLECULAR WEIGHT:AMB[G],WTMOLB[G/GMOLE]
6678. 18.5

UNIVERSAL GAS CONSTANT: RU[PSI*ML/GMOLE/K],ATM PRESS[PSIA]
1205.95 14.696

SOL-GAS INFO: VOL FRACT (VFRG),MOL WT(WTMOLG),CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
4

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-03	504	2123.9	2117.5	30.5	20.25	4.07
-04	3169	2132.6	2126.1	30.8	26.9	2.16
-05	5752	2137.9	2131.4	31.4	28.8	2.08
-06	8323	2128.0	2121.6	30.9	27.3	2.10

PXD BACKFILL INFO:[NO,PT NO],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-02	2957	2130.5	2131.3	30.6	30.6	27.0	2.14
-----	------	--------	--------	------	------	------	------

-03	7428	2128.6	2127.9	31.0	31.0	28.3	2.00
-04	11632	2132.4	2132.6	31.4	31.4	30.2	1.93
-05	15981	2105.0	2105.3	29.8	29.8	20.6	3.90
-06	20240	2119.2	2120.6	30.5	30.5	24.6	2.60
-07	24409	2059.1	2058.7	25.0	25.0	19.9	4.20

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS: NPTK, PK, TRTDK, TGBK, TEXK
 24385 2103.8 29.1 20.0 4.15

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

24428 2058.0 25.0 21.1 3.70

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS: PK, TRTDK, TGBK, TEXK

23607 2121.8 30.1 26.2 2.27

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

23646 2202.2 37.0 26.2 2.27

NUMBER OF DATA POINTS TO BE ADJUSTED & INPUT DATA TYPE, ISTRM

3 1

DATA-PT NO., DATE&TIME, PRESS, RTD TEMP, GB TEMP, EXCESS TEMP

8001	03-17-97:22	2130.8	31.0	28.7	1.97
14001	11-29-97:01	2109.5	30.0	22.1	3.33
20001	08-09-98:08	2120.0	30.4	24.9	2.53

TC-161 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PXD CALIBRATIONS: NCALT,NCALP
8 6

RTD CALIBRATION INFORMATION: [DATE&HR],PT NO.,COMP,RESIDT

02-12-96:??	1	0.	0.
07-15-96:??	3323	0.5	0.
01-13-97:??	7558	0.	0.
07-09-97:??	11626	0.	0.1
11-21-97:??	14848	0.6	0.1
05-21-98:??	19142	-0.9	0.
11-21-98:??	23524	0.4	0.
05-24-99:??	27711	0.	-0.1

PXD CALIBRATION INFO: [DATE&HR],PT NO,COMP,RESIDP

08-13-96:10	3970	0.	0.
02-24-97:??	8513	0.	0.
08-21-97:??	12652	0.	0.
02-20-98:??	17002	0.	0.
08-19-98:??	21268	0.	0.
02-17-99:??	25433	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2098.1 31.2 28.6 1.98

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.17 0.19

BRINE MASS & MOLECULAR WEIGHT: AMB[G],WTMOLB[G/GMOLE]
6872. 18.5

UNIVERSAL GAS CONSTANT: RU[PSI*ML/GMOLE/K],ATM PRESS[PSIA]
1205.95 14.696

SOL GAS INFO: VOL FRACT[VFRG],MOL WT (WTMOLG), CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
5

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTDS,TGBS,TGBEXS

-02	105	2205.6	2197.2	34.6	27.5	2.13
-03	1518	2105.6	2097.6	30.0	20.0	4.20
-04	4178	2099.0	2091.5	30.1	26.9	2.16
-05	6756	2110.1	2102.7	31.2	28.65	1.98
-06	9358	2098.5	2091.3	30.8	28.3	2.00

PXD BACKFILL INFO:[NO,PT NO],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-02	3970	2099.3	2099.3	30.2	30.2	27.0	2.14
-03	8513	2097.9	2098.8	30.9	30.9	28.4	2.00
-04	12652	2104.0	2104.2	31.1	31.1	30.2	1.93
-05	17002	2082.9	2083.3	30.3	30.3	20.6	3.90
-06	21268	2097.2	2098.8	30.3	30.3	24.6	2.60
-07	25433	2076.8	2076.4	29.2	29.2	19.9	4.20

BETA DETERMINATION POINTS: NBETA

2

FIRST (LO-TEMP) BETA-PT. REF. CONDITIONS:NPTK,PK,TRTDK,TGBK,TEXK
 25574 2074.1 29.1 20.8 3.82

BETA-POINT STEP CONDITIONS:NPTB,PB,TRTDB,TGBB,TEXB
 25604 2027.6 25.3 20.8 3.82

SECOND (HI-TEMP) BETA-PT.REF.CONDITIONS:NPTK,PK,TRTDK,TGBK,TEXK
 23385 2099.0 30.2 25.9 2.32

BETA-POINT STEP CONDITIONS:NPTB,PB,TRTDB,TGBB,TEXB
 23450 2158.0 34.8 25.9 2.32

NUMBER OF DATA POINTS TO BE ADJUSTED & INPUT DATA TYPE, ISTRM

3 1

DATA-PT NO.	DATE&TIME	PRESS	RTD TEMP	GB TEMP	EXCESS TEMP
8001	02-01-97:11		2101.3	31.2	28.8 1.97
14001	10-16-97:22		2110.7	31.9	29.6 1.93
20001	06-26-98:19		2074.9	28.9	21.9 3.40

TC-161e Set-up (Using empirical RTD calibration factors)

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PXD CALIBRATIONS: NCALT,NCALP
8 6

RTD CALIBRATION INFORMATION: [DATE&HR],PT NO.,COMP,RESIDT

02-12-96:??	1	0.	0.
07-15-96:??	3323	0.8	0.
01-13-97:??	7558	0.3	-0.1
07-09-97:??	11626	-0.35	0.45
11-21-97:??	14848	0.6	0.
05-21-98:??	19142	-0.7	0.7
11-21-98:??	23524	0.6	-0.1
05-24-99:??	27711	0.1	0.

PXD CALIBRATION INFO: [DATE&HR],PT NO,COMP,RESIDP

08-13-96:10	3970	0.	0.
02-24-97:??	8513	0.	0.
08-21-97:??	12652	0.	0.
02-20-98:??	17002	0.	0.
08-19-98:??	21268	0.	0.
02-17-99:??	25433	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2098.1 31.2 28.6 1.98

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.17 0.19

BRINE MASS & MOLECULAR WEIGHT: AMB[G],WTMOLB[G/GMOLE]
6872. 18.5

UNIVERSAL GAS CONSTANT: RU[PSI*ML/GMOLE/K],ATM PRESS[PSIA]
1205.95 14.696

SOL GAS INFO: VOL FRACT[VFRG],MOL WT (WTMOLG), CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
5

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTDS,TGBS,TGBEXS

-02	105	2205.6	2197.2	34.6	27.5	2.13
-03	1518	2105.6	2097.6	30.0	20.0	4.20
-04	4178	2099.0	2091.5	30.1	26.9	2.16
-05	6756	2110.1	2102.7	31.2	28.65	1.98
-06	9358	2098.5	2091.3	30.8	28.3	2.00

PXD BACKFILL INFO:[NO,PT NO],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-02	3970	2099.3	2099.3	30.2	30.2	27.0	2.14
-03	8513	2097.9	2098.8	30.9	30.9	28.4	2.00
-04	12652	2104.0	2104.2	31.1	31.1	30.2	1.93
-05	17002	2082.9	2083.3	30.3	30.3	20.6	3.90
-06	21268	2097.2	2098.8	30.3	30.3	24.6	2.60
-07	25433	2076.8	2076.4	29.2	29.2	19.9	4.20

BETA DETERMINATION POINTS: NBETA

2

FIRST (LO-TEMP) BETA-PT. REF. CONDITIONS:NPTK,PK,TRTDK,TGBK,TEXK
 25574 2074.1 29.1 20.8 3.82

BETA-POINT STEP CONDITIONS:NPTB,PB,TRTDB,TGBB,TEXB
 25604 2027.6 25.3 20.8 3.82

SECOND (HI-TEMP) BETA-PT.REF.CONDITIONS:NPTK,PK,TRTDK,TGBK,TEXK
 23385 2099.0 30.2 25.9 2.32

BETA-POINT STEP CONDITIONS:NPTB,PB,TRTDB,TGBB,TEXB
 23450 2158.0 34.8 25.9 2.32

NUMBER OF DATA POINTS TO BE ADJUSTED & INPUT DATA TYPE, ISTRM

3 1

DATA-PT NO.	DATE&TIME	PRESS	RTD TEMP	GB TEMP	EXCESS TEMP
8001	02-01-97:11		2101.3	31.2	28.8 1.97
14001	10-16-97:22		2110.7	31.9	29.6 1.93
20001	06-26-98:19		2074.9	28.9	21.9 3.40

TC-162 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PXD CALIBRATIONS: NCALT,NCALP
8 7

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	1	0.	0.
07-15-96:??	3030	0.	0.
01-13-97:??	7260	0.	0.
07-09-97:??	11320	0.	0.
11-21-97:??	14528	0.	0.
05-21-98:??	18804	0.	-0.1
11-23-98:??	23162	0.	0.
05-24-99:??	27331	0.	0.

PXD CALIBRATIONS [DATE:HR],PT NO,COMP,RESIDP

03-01-96:11	18	0.	0.
08-13-96:11	3677	-0.75	0.
02-21-97:??	8143	0.	0.
08-21-97:??	12339	0.	0.
02-20-98:??	16674	0.	0.
08-19-98:??	20925	0.	0.
02-17-99:??	25071	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2090.3 30.7 28.4 2.00

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.17 0.19

BRINE MASS AND MOLECULAR WT: AMB [G],WTMOLB [G/GMOLE]
6891. 18.5

UNIVERSAL GAS CONSTANT: RU [PSI*ML/GMOLE/K],ATM PRESS [PSIA]
1205.95 14.696

SOL GAS INFO: VOL FRACT[VFRG],MOL WT[WTMOLG],CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
6

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-03	20	2155.2	2147.4	30.1	27.2	2.12
-04	107	2142.0	2134.8	29.9	26.15	2.27
-05	1447	2107.3	2099.1	30.1	20.15	4.11
-06	3982	2110.0	2102.4	30.7	27.25	2.12
-07	6656	2113.4	2105.8	31.4	28.7	1.97

-08	9168	2097.9	2090.5	30.7	28.35	1.99	
PXD BACKFILL INFO: [NO,PT NO],PC1,PC2,TC1,TC2,TGBC,TGBEXC							
-01	18	2152.0	2152.17	29.9	29.9	27.2	2.12
-02	3677	2115.0	2111.5	30.7	30.7	27.0	2.14
-03	8143	2097.8	2097.3	30.9	30.9	28.5	1.99
-04	12339	2096.7	2097.4	31.1	31.1	29.2	1.95
-05	16674	2070.1	2069.5	29.5	29.5	20.6	3.90
-06	20925	2081.8	2081.8	30.4	30.4	24.6	2.60
-07	25071	2073.7	2073.4	29.7	29.7	19.9	4.20
BETA DETERMINATION POINTS: NBETA							
2							
FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS:NPTK,PK,TRTDK,TGBK,TEXK							
24795		2073.2		29.7	21.1	3.70	
BETA-POINT STEP CONDITIONS:PB,TRTDB,TGBB,TEXB							
24831		2034.1		26.6	20.8	3.82	
SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS:PK,TRTDK,TGBK,TEXK							
24441		2088.1		30.6	26.3	2.25	
BETA-POINT STEP CONDITIONS: PB,TRTDB,TGBB,TEXB							
24470		2166.9		36.9	23.9	2.77	
NUMBER OF DATA POINTS TO BE ADJUSTED AND INPUT DATA KEY, ISTRM							
3 1							
DATA-PT NO.,DATE&TIME,PRESS,RTD TEMP,GB TEMP,EXCESS TEMP							
8001	02-15-97:08		2100.3	31.0	28.7	1.97	
14001	10-30-97:05		2069.4	29.2	24.2	2.69	
20001	07-11-98:08		2076.0	29.9	22.9	3.07	

TC-163 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PXD CALIBRATIONS: NCALT, NCALP
8 6

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	1	0.	-0.1
07-15-96:??	2729	0.	-0.1
01-13-97:??	6968	0.	-0.1
07-09-97:??	11008	0.	0.
11-21-97:??	14220	-0.1	0.
05-21-98:??	18497	0.	-0.1
11-23-98:??	22857	0.	0.
05-24-99:??	27030	0.	0.1

PRESSURE XDUCR CALIBRATIONS: [DATE:HR],PT NO,COMP,RESIDP

05-20-96:??	1561	0.	0.
11-14-96:??	5581	0.	0.
05-14-97:??	9698	0.	0.
12-02-97:??	14473	0.	0.
06-01-98:??	18754	0.	0.
12-01-98:??	23041	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2173.0 31.0 28.5 1.99

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.17 0.19

BRINE MASS & MOLECULAR WT: AMB [G],WTMOLB [G/GMOLE]
7708. 18.5

UNIVERSAL GAS CONSTANT: RU [PSI*ML/GMOLE/K], ATM PRESS [PSIA]
1205.95 14.696

SOL GAS INFO: VOL FRACT [VFRG],MOL WT[WTMOLG], CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
5

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-05	1472	2174.7	2166.9	29.8	20.4	3.98
-07	1616	2192.9	2185.2	29.8	21.5	3.55
-08	4090	2187.5	2180.0	30.7	27.5	2.08
-09	7032	2187.9	2180.4	31.1	28.7	1.97
-10	9580	2172.3	2164.9	30.4	28.2	2.01

PXD BACKFILL INFO: [NO,PT NO],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	1561	2130.9	2130.9	24.2	24.2	19.8	4.24
-02	5581	2184.4	2184.4	31.0	31.0	28.3	2.00
-03	9698	2169.5	2170.1	30.7	30.7	28.4	2.00
-04	14473	2157.2	2156.4	30.1	30.1	22.1	3.33
-05	18754	2148.2	2148.2	29.8	29.8	19.2	4.52
-06	23041	2161.3	2161.3	30.3	30.4	26.1	2.28

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS: NPTK, PK, TRTDK, TGBK, TEXK

24626	2151.5	29.7	20.4	3.98
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

24661	2104.5	26.1	20.3	4.02
-------	--------	------	------	------

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS: PK, TRTDK, TGBK, TEXK

23758	2166.2	30.5	26.1	2.28
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

23777	2255.5	37.25	26.1	2.27
-------	--------	-------	------	------

NUMBER OF DATA POINTS TO BE ADJUSTED AND INPUT TYPE KEY, ISTRM

3 1

DATA-PT NO., DATE&TIME, PRESS, RTD TEMP, GB TEMP, EXCESS TEMP

8001	02-27-97:22	2177.4	30.7	28.6	1.98
14001	11-12-97:04	2141.8	28.8	22.4	3.23
20001	07-24-98:11	2160.8	30.3	23.8	2.80

TC-164 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PXD CALIBRATIONS: NCALT,NCALP
8 5

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	0	0.	0.
07-15-96:??	1962	0.	0.
01-13-97:??	6762	0.	0.
07-09-97:??	10817	0.	0.1
11-21-97:??	14037	0.	0.
05-21-98:??	18232	0.	-0.1
11-23-98:??	22596	0.	0.
05-24-99:??	26743	0.	0.

PRESSURE XDUCR CALIBRATIONS: [DATE:HR],PT NO,COMP,RESIDP

12-05-96:??	5875	0.	0.
06-05-97:??	10007	0.	0.
12-02-97:??	14290	0.	0.
06-01-98:??	18494	0.	0.
12-01-98:??	22781	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTD,GBP,TGBEXP

10001	2167.1	30.7	28.3	2.00
-------	--------	------	------	------

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI

50	0.17	0.19
----	------	------

BRINE MASS AND MOLECULAR WT: AMB [G], WTMOLB [G/GMOLE]

7708.	18.5
-------	------

UNIVERSAL GAS CONSTANT: RU [PSI*ML/GMOLE/K],ATM PRESS[PSIA]

1205.95	14.696
---------	--------

SOL GAS INFO: VOL FRACT[VFRG],MOL WT[WTMOLG],CONSTANTS A,B,C

0.	-67.3877	86.3213	24.7981
----	----------	---------	---------

SAMPLE VOLUME: VSAMPL

3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL

5

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-02	100	2220.3	2213.3	30.1	20.7	3.90
-03	1409	2183.4	2175.6	30.85	20.9	3.82
-04	3871	2184.2	2176.3	30.6	27.5	2.08
-05	6804	2186.2	2178.4	31.1	28.7	1.97
-06	9361	2172.0	2164.1	30.6	27.75	2.04

PXD BACKFILL INFO: [NO,PT NO],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	5875	2185.8	2188.4	31.1	31.1	28.6	1.98
-----	------	--------	--------	------	------	------	------

-02	10007	2166.9	2167.8	30.7	30.7	28.3	2.00
-03	14290	2155.8	2156.2	30.2	30.2	22.1	3.33
-04	18494	2148.8	2148.9	29.9	29.9	19.2	4.52
-05	22781	2157.9	2160.0	30.5	30.3	26.1	2.28

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS: NPTK, PK, TRTDK, TGBK, TEXK
 24468 2140.3 29.3 20.0 4.15

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

24506 2089.8 25.3 21.2 3.66

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS: PK, TRTDK, TGBK, TEXK

23700 2161.8 30.5 26.2 2.27

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

23729 2251.1 37.2 26.2 2.27

NUMBER OF DATA POINTS TO BE ADJUSTED & INPUT DATA KEY, ISTRM

3 1

DATA-PT NO., DATE&TIME, PRESS, RTD TEMP, GB TEMP, EXCESS TEMP

8001	03-08-97:16	2176.2	30.9	28.6	1.98
14001	11-19-97:22	2143.1	29.2	22.5	3.19
20001	08-04-98:16	2153.5	30.0	24.1	2.72

TC-165 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PRESS-XDUCER CALIBRATIONS: NCALT,NCALP
8 6

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	0	0.	0.
07-15-96:??	2537	0.	0.
01-13-97:??	6776	0.	0.
07-09-97:??	10836	0.	0.1
11-21-97:??	14045	0.	0.
05-21-98:??	18323	0.	-0.1
11-23-98:??	22682	0.	0.
05-24-99:??	26842	0.	0.1

PRESSURE-XDUCER CALIBRATION INFO: [DATE:HR],PT NO.,COMP.,RESIDP

09-19-96:09	4066	0.	0.
03-19-97:??	8264	0.	0.
09-19-97:??	12546	0.	0.
02-20-98:??	16195	0.	0.
08-19-98:??	20439	0.	0.
02-17-99:??	24582	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP

10001	2142.0	30.6	28.4	2.00
-------	--------	------	------	------

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI

50	0.17	0.19
----	------	------

BRINE MASS AND MOLECULAR WEIGHT: AMB [G],WTMOLB [G/GMOLE]

7708.	18.5
-------	------

UNIVERSAL GAS CONSTANT: RU [PSI*ML/GMOLE/K], ATM PRESS [PSIA]

1205.95	14.696
---------	--------

SOL GAS INFO: VOL FRACT[VFRG],MOL WT[WTMOLG],CONSTANTS A,B,C

0.	-67.3877	86.3213	24.7981
----	----------	---------	---------

SAMPLE VOLUME: VSAMPL

3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL

5

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-02	106	2207.9	2199.7	30.5	21.55	3.55
-03	1391	2152.8	2144.0	30.05	21.15	3.70
-04	3879	2162.1	2153.1	30.65	27.55	2.08
-05	6839	2161.8	2152.8	31.1	28.55	1.99
-06	9381	2147.4	2138.4	30.6	27.3	2.09

PXD BACKFILL INFO: [NO.,PT.NO.],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	4066	2152.9	2152.9	30.6	30.6	27.4	2.09
-02	8264	2154.4	2155.9	31.1	31.1	28.8	1.97
-03	12546	2153.1	2153.2	31.4	31.4	29.5	1.94
-04	16195	2118.4	2117.9	29.7	29.7	20.6	3.90
-05	20439	2130.6	2130.5	30.2	30.2	24.6	2.60
-06	24582	2114.8	2114.4	29.3	29.4	19.9	4.20

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS: NPTK, PK, TRTDK, TGBK, TEXK

24443	2115.0	29.4	20.4	3.98
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

24477	2068.8	25.9	20.3	4.02
-------	--------	------	------	------

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS: PK, TRTDK, TGBK, TEXK

25036	2114.4	29.3	22.9	3.07
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

25054	2205.7	35.8	23.0	3.03
-------	--------	------	------	------

NUMBER OF DATA POINTS TO BE ADJUSTED AND INPUT TYPE KEY, ISTRM

3 1

DATA-PT NO., DATE&TIME, PRESS, RTD TEMP, GB TEMP, EXCESS TEMP

8001	03-07-97:21	2151.5	30.9	28.6	1.98
14001	11-19-97:12	2115.9	29.1	22.5	3.19
20001	07-31-98:22	2128.7	30.1	24.0	2.75

TC-166 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PXD CALIBRATIONS: NCALT,NCALP
8 7

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	1	0.	-0.1
07-15-96:??	2280	0.	-0.1
01-13-97:??	6520	0.	0.1
07-09-97:??	10580	0.	0.1
11-21-97:??	13799	0.	0.
05-21-98:??	18070	0.	0.
11-23-98:??	22431	0.	0.1
05-24-99:??	26400	0.	0.1

PRESSURE-XDUCER CALIBRATION INFO:[DATE:HR],PT NO,COMP,RESIDP

04-01-96:??	1	0.	0.
06-13-96:??	1664	0.	0.
12-05-96:??	5628	0.	0.
06-05-97:??	9773	0.	0.
12-02-97:??	14052	0.	0.
06-01-98:??	18329	0.	0.
12-01-98:??	22434	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2152.7 31.0 28.6 1.98

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.17 0.19

BRINE MASS AND MOLECULAR WEIGHT: AMB[G],WTMOLB[G/GMOLE]
7548. 18.5

UNIVERSAL GAS CONSTANT: RU[PSI*ML/GMOLE/K], STD ATM PRESS[PSIA]
1205.95 14.696

SOLUBLE-GAS INFO:VFRG(VOL FRACT),WTMOLG(MOL WT),CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
5

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-02	26	2197.4	2188.1	30.9	21.4	3.58
-03	1490	2168.3	2158.9	30.6	22.2	3.29
-04	3948	2161.4	2152.2	30.3	27.6	2.07
-05	6675	2168.8	2159.3	31.2	28.5	1.99
-06	9241	2151.6	2142.5	30.5	28.3	2.00

PXD BACKFILL INFO:[NO,PT],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	1	2130.2	2130.2	25.5	25.5	20.5	3.94
-02	1664	2156.9	2156.9	30.5	30.5	21.6	3.51
-03	5628	2165.4	2166.9	31.0	31.0	28.6	1.98
-04	9773	2145.8	2146.3	30.6	30.6	27.7	2.06
-05	14052	2145.5	2145.0	30.7	30.7	22.1	3.33
-06	18329	2145.0	2145.0	30.7	30.7	19.5	4.38
-07	22434	2164.4	2166.5	30.5	30.6	26.0	2.30

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS:NPTK,PK,TRTDK,TGBK,TEXK

24288	2137.5	28.8	20.8	3.82
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS:PB,TRTDB,TGBB,TEXB

24311	2092.3	25.4	20.8	3.82
-------	--------	------	------	------

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS:PK,TRTDK,TGBK,TEXK

22124	2162.9	30.5	25.8	2.34
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB,TRTDB,TGBB,TEXB

22142	2226.1	35.1	25.8	2.34
-------	--------	------	------	------

NUMBER OF DATA POINTS TO BE ADJUSTED AND FILE KEY (=0, THIS FILE)

3 0

DATA-PT NO.,DATE&TIME,PRESS,RTD TEMP,GB TEMP,EXCESS TEMP

8001	03-19-97:03	2156.8	31.0	28.7	1.97
14001	11-30-97:03	2143.0	30.7	22.0	3.36
20001	08-11-98:16	2155.9	30.5	24.9	2.53

TC-167 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PXD CALIBRATIONS: NCALT,NCALP
8 6

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	0	0.	-0.1
07-15-96:??	2148	0.	-0.1
01-13-97:??	6399	0.	0.
07-09-97:??	10450	0.	0.1
11-21-97:??	13666	0.	0.
05-21-98:??	17946	0.	0.1
11-23-98:??	22312	0.	0.
05-24-99:??	26488	0.	0.

PRESSURE XDUCR CALIBRATION INFO: [DATE:HR],PT NO,COMP,RESIDP

04-08-96:14	1	0.	0.
10-03-96:??	4006	0.	0.
04-03-97:??	8230	0.	0.
12-01-97:??	13899	0.	0.
06-01-98:??	18207	0.	0.
12-01-98:??	22499	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2169.6 31.2 28.8 1.97

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.17 0.19

BRINE MASS AND MOLECULAR WEIGHT: AMB[G],WTMOLB[G/GMOLE]
7161. 18.5

UNIVERSAL GAS CONSTANT: RU[PSI*ML/GMOLE/K],STD ATM PRESS[PSIA]
1205.95 14.696

SOL-GAS INFO: VFRG(VOL FRACT),WTMOLG(MOL WT),CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
5

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-02	45	2204.8	2197.3	30.15	21.65	3.51
-03	1461	2174.5	2166.5	30.3	21.9	3.44
-04	3964	2183.1	2175.1	30.8	27.9	2.04
-05	6627	2179.6	2171.7	31.0	28.35	1.99
-06	9129	2169.0	2161.2	30.65	28.1	2.00

PXD BACKFILL INFO: [NO,PT NO],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	1	2135.2	2135.2	23.9	23.9	21.9	3.40
-02	4006	2174.8	2172.4	30.8	30.8	27.9	2.04
-03	8230	2167.6	2167.6	30.7	30.7	27.8	2.05
-04	13899	2150.2	2150.1	30.1	30.1	22.0	3.36
-05	18207	2146.7	2146.7	29.9	29.9	19.5	4.38
-06	22499	2157.0	2159.1	30.0	30.1	26.0	2.30

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS: NPTK, PK, TRTDK, TGBK, TEXK
 18742 2148.0 30.0 21.6 3.51

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

18765 2112.1 27.1 21.6 3.51

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS: PK, TRTDK, TGBK, TEXK

23718 2150.5 29.6 22.1 3.33

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

23742 2241.5 36.6 22.0 3.36

NUMBER OF DATA POINTS TO BE ADJUSTED & READ KEY (=0: THIS FILE)

3 1

DATA-PT NO., DATE&TIME, PRESS, RTD TEMP, GB TEMP, EXCESS TEMP

8001	03-24-97:15	2169.9	30.9	28.5	1.99
14001	12-06-97:04	2151.0	30.2	21.7	3.47
20001	08-16-98:18	2153.3	30.1	24.7	2.57

TC-168 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PXD CALIBRATIONS: NCALT,NCALP
8 6

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	0	0.	0.
07-15-96:??	2057	0.	-0.1
01-13-97:??	6305	0.	0.
07-09-97:??	10368	0.	0.
11-21-97:??	13576	-0.1	0.
05-21-98:??	17830	0.	0.1
11-23-98:??	22187	0.	0.
05-24-99:??	26376	0.	0.1

PRESSURE-XDUCR CALIBRATION INFO: [DATE:HR],PT NO,COMP,RESIDP

04-15-96:??	69	0.	0.
10-03-96:??	3919	0.	0.
04-03-96:??	8148	0.	0.
12-01-97:??	13808	0.	0.
06-01-98:??	18093	0.	0.
12-01-98:??	22373	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2146.5 31.3 28.9 1.96

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.17 0.19

BRINE MASS AND MOLECULAR WEIGHT: AMB[G],WTMOLB[G/GMOLE]
7416. 18.5

UNIVERSAL GAS CONSTANT: RU[PSI*ML/GMOLE/K],STD ATM PRESS[PSIA]
1205.95 14.696

SOL-GAS INFO:VFRG(VOL FRACT),WTMOLG(MOL WT),CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
5

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-02	118	2184.3	2176.6	30.1	21.2	3.66
-03	1462	2154.8	2147.2	29.8	22.4	3.26
-04	4015	2161.4	2153.5	30.4	28.0	2.03
-05	6864	2154.7	2146.9	30.8	28.5	1.98
-06	9394	2147.9	2140.1	30.9	28.3	2.00

PXD BACKFILL INFO: [NO.,PT NO],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	69	2104.5	2104.6	23.3	23.3	20.3	4.02
-02	3919	2158.9	2161.9	30.4	30.4	27.9	2.04
-03	8148	2141.9	2142.1	30.7	30.7	27.8	2.05
-04	13808	2120.4	2120.4	29.8	29.8	22.0	3.36
-05	18093	2111.5	2114.2	29.5	29.5	19.5	4.38
-06	22373	2125.8	2128.1	30.1	30.2	26.0	2.30

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS: NPTK, PK, TRTDK, TGBK, TEXK

23962	2113.3	29.5	20.4	3.98
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

23990	2064.2	25.5	20.4	3.98
-------	--------	------	------	------

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS: PK, TRTDK, TGBK, TEXK

23726	2115.2	29.6	21.4	3.58
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXB

23746	2210.6	36.9	21.3	3.62
-------	--------	------	------	------

NUMBER OF DATA POINTS TO BE ADJUSTED & DATA KEY (0=THIS FILE)

3 1

DATA-PT NO., DATE&TIME, PRESS, RTD TEMP, GB TEMP, EXCESS TEMP

8001	03-28-97:06	2148.3	31.0	28.7	1.97
14001	12-09-97:22	2120.0	30.0	21.5	3.55
20001	08-22-98:02	2125.5	30.3	25.1	2.48

TC-169 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD AND PRESSURE XDUCER CALIBRATIONS: NCALT,NCALP
8 5

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	0	0.	0.1
07-15-96:??	1749	0.	0.1
01-13-97:??	5997	0.	0.
07-09-97:??	10053	0.	0.1
11-21-97:??	13266	0.1	0.
05-21-98:??	17550	0.	0.1
11-23-98:??	21920	0.	0.1
05-24-98:??	26101	0.	0.1

PRESSURE-XDUCER CALIBRATION INFO: [DATE:HR],PT NO,COMP,RESIDP

10-03-96:??	3608	0.	0.
04-03-97:??	7841	0.	0.
12-02-97:??	13521	0.	0.
06-01-98:??	17809	0.	0.
12-01-98:??	22108	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTD, TGBP, TGBEXP

10001	2172.8	30.1	28.2	2.01
-------	--------	------	------	------

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI

50	0.17	0.19
----	------	------

BRINE MASS AND MOLECULAR WEIGHT: AMB[G],WTMOLB[G/GMOLE]
7472. 18.5

UNIVERSAL GAS CONSTANT: RU[PSI(ML/GMOLE/K),STD ATM PRESS[PSIA]
1205.95 14.696

SOL-GAS INFO: VFRG(VOL FRACT),WTMOLG(MOL WT),CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
4

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-02	136	2196.1	2187.3	30.0	20.25	4.07
-03	2706	2198.1	2189.6	30.5	27.35	2.09
-04	5389	2203.4	2195.0	31.1	28.85	1.97
-05	7901	2188.4	2180.0	30.7	27.9	2.04

PXD BACKFILL INFO:[NO,PT NO,],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	3608	2192.0	2195.8	30.6	30.6	27.7	2.06
-02	7841	2184.9	2184.7	30.5	30.5	27.2	2.12

-03	13521	2167.1	2166.9	30.1	30.1	22.1	3.33
-04	17809	2160.1	2161.7	29.9	29.9	19.5	4.38
-05	22108	2170.6	2172.2	30.2	30.2	26.0	2.30

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS: NPTK, PK, TRTDK, TGBK, TEXK

23543	2158.5	29.5	21.2	3.66
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXTB

23596	2109.3	25.8	20.8	3.82
-------	--------	------	------	------

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS: PK, TRTDK, TGBK, TEXK

23194	2171.7	30.2	26.3	2.25
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB, TRTDB, TGBB, TEXTB

23223	2267.7	37.3	23.9	2.77
-------	--------	------	------	------

NUMBER OF DATA POINTS TO BE ADJUSTED AND INPUT KEY (THIS FILE=0)

3 1

DATA-PT NX., DATE&TIME, PRESS, RTD TEMP, GB TEMP, EXCESS TEMP

8001	04-12-97:18	2180.3	30.8	28.5	1.99
14001	12-22-97:16	2160.8	29.8	21.1	3.70
20001	09-02-98:12	2170.3	30.3	25.2	2.46

TC-170 Setup

LENGTHS OF VARIOUS REGIONS: L0,L1,L2,L3,L4,L5,L6

0.03795 0.04440 0.04260 0.09070 0.0

0.36154 0.36154

ARGON GAS DATA: NAR/TAR,AKAR,VAR,CAR,RAR

3

-23.16 0.0152 1.196E-5 520.3 1.630

26.84 0.0177 1.686E-5 520.3 1.358

126.84 0.0223 2.836E-5 520.3 1.019

TC HEAD DATA: NHD/THD,AKHD,VHD,CHD,RHD

1

25.0 12.55

HEADSPACE-GAS DATA: NHS/THS,AKHS,VHS,CHS,RHS

3

-23.16 0.0222 0.778E-7 1038.3 200.4

26.84 0.026 1.078E-7 1040.8 167.0

126.84 0.0325 1.785E-7 1045.9 124.9

BRINE/WASTE DATA: NBW/TBW,AKBW,VBW,CBW,RBW

4

0. 0.501 1.441E-6 3399.4 1243.6

20. 0.597 0.8162E-6 3393.0 1233.1

40. 0.628 0.5356E-6 3401.1 1221.9

60. 0.651 0.3893E-6 3408.0 1210.0

CYCLE LIMIT AND TEMPERATURE CONVERGENCE TOLERANCE: LIMIT, DTERR

100 0.001

WATER-VAPOR PRESSURE TABLE

21

1 20. 0.023388

2 21. 0.024877

3 22. 0.026447

4 23. 0.028104

5 24. 0.029850

6 25. 0.031691

7 26. 0.033629

8 27. 0.035670

9 28. 0.037818

10 29. 0.040078

11 30. 0.042455

12 31. 0.044953

13 32. 0.047578

14 33. 0.050335

15 34. 0.053229

16 35. 0.056267

17 36. 0.059454

18 37. 0.062795

19	38.	0.066298
20	39.	0.069969
21	40.	0.073814

TEST-CONTAINER VOLUME & LINEAR THERMAL-EXPANSION COEFFICIENT
7272. 11.3E-6

GLOBAL EXCESS TEMP OF GB INTERIOR VS. THE GB RTD MEASUREMENT
0.

NUMBER OF RTD & PRESS XDUCER CALIBRATIONS: NCALT,NCALP
8 7

RTD CALIBRATION INFORMATION: [DATE:HR],PT NO.,COMP,RESERR

11-03-95:??	0	0.	0.1
07-15-96:??	1233	0.	0.1
01-13-97:??	5481	0.	0.
07-09-97:??	9544	0.	0.1
11-21-97:??	12758	-0.1	0.
05-21-98:??	17044	0.	0.1
11-23-98:??	21413	0.	0.1
05-24-99:??	25578	0.	0.2

PRESSURE XDUCER CALIBRATION INFO:[DATE:HR],PT NO,COMP,RESIDP

05-15-96:??	21	0.	0.
05-31-96:??	324	0.	0.
11-14-96:??	4095	0.	0.
05-14-97:??	8227	0.	0.
12-02-97:??	13012	0.	0.
06-02-98:??	17320	0.	0.
12-07-98:??	21737	0.	0.

OVERALL REFERENCE PT DATA: NPTP,PP,TRTDP,TGBP,TGBEXP
10001 2160.8 31.0 29.1 1.95

HS-GAS COMPRESSIBILITY TABLE DATA: NUM,VLO,VHI
50 0.17 0.19

BRINE MASS AND MOLECULAR WEIGHT: AMB[G],WTMOLB[G/GMOLE]
7638. 18.5

UNIVERSAL GAS CONSTANT: RU[PSI*ML/GMOLE/K],STD ATM PRESS[PSIA]
1205.95 14.696

SOL-GAS INFO: VFRG (VOL FRACT),WTMOLG (MOL WT),CONSTANTS A,B,C
0. -67.3877 86.3213 24.7981

SAMPLE VOLUME: VSAMPL
3.05

NUMBER OF GAS-SAMPLE DATA POINTS: NSAMPL
5

GAS-SAMPLE DATA:[ID],NPTS(I),PS1,PS2,TRTD,TGB,TGBEX

-02	45	2205.4	2195.6	30.5	21.4	3.55
-04	419	2188.4	2178.6	30.2	22.2	3.29
-05	2907	2178.9	2169.3	30.5	27.6	2.07
-06	5570	2184.1	2174.5	31.4	28.5	1.99
-07	8184	2159.4	2150.0	30.55	27.6	2.07

PXD BACKFILL INFO:[NO.,PT NO.],PC1,PC2,TC1,TC2,TGBC,TGBEXC

-01	21	2126.7	2126.7	23.2	23.2	21.2	3.66
-02	324	2165.0	2165.0	30.7	30.7	19.9	4.20
-03	4095	2172.2	2174.6	30.7	30.7	28.3	2.00
-04	8227	2152.1	2152.8	30.5	30.5	27.8	2.05
-05	13012	2138.6	2138.8	30.0	30.0	22.1	3.33
-06	17320	2132.7	2133.1	29.9	29.9	19.6	4.33
-07	21737	2147.9	2149.1	30.5	30.5	25.9	2.32

BETA DETERMINATION POINTS: NBETA

2

FIRST (LOW TEMP) BETA-PT. REF. CONDITIONS:NPTK,PK,TRTDK,TGBK,TEXK

12050	2171.7	31.75	29.8	1.93
-------	--------	-------	------	------

BETA-POINT STEP CONDITIONS:PB,TRTDB,TGBB,TEXB

12089	2137.35	29.65	25.9	2.32
-------	---------	-------	------	------

SECOND (HIGH TEMP) BETA-PT. REF. CONDITIONS:PK,TRTDK,TGBK,TEXK

22811	2128.6	29.3	22.1	3.33
-------	--------	------	------	------

BETA-POINT STEP CONDITIONS: PB,TRTDB,TGBB,TEXB

22837	2225.7	36.1	22.1	3.33
-------	--------	------	------	------

NUMBER OF DATA POINTS TO BE ADJUSTED AND INPUT KEY (0=THIS FILE)

3 1

DATA-PT NO.,DATE&TIME,PRESS,RTD TEMP,GB TEMP,EXCESS TEMP

8001	05-04-97:23	2161.5	30.7	28.4	2.00
14001	01-13-98:05	2135.5	30.0	20.9	3.78
20001	09-24-98:02	2150.0	30.8	25.6	2.38

ATTACHMENT 2 TO APPENDIX D

Streaming-Data-Input Procedure

(Rev. 03-2002)

1. Add most current data to the EXCEL data file (on the S: drive).
2. Copy GGE Project-generated EXCEL spreadsheet (on the S: drive) to ADJxxx.xls, where xxx denotes the TC number (e.g., 153), for later manipulation.
3. Make the following adjustments to this new EXCEL copy:
 - a. Make sure that all data are floating points
 - b. Check that column widths are the standard default of 8.43
 - c. Delete the “DateValue” column (1st column - A)
 - d. Format T_{RTD} , T_{GB} , and Pressure column to 1 decimal place
 - e. Make T_{excess} calculation, per desired algorithm, and place in 6th column (F), formatted to 2 decimal places
 - f. Set flags in next 2 columns (G & H) for
 - (a) Col. G: duplicate data (time): 1=TRUE; 0=FALSE -- IF(B2=B1,1,0)
 - (b) Col. H: dropped data: 1=TRUE; 0=FALSE -- IF(OR(C2=0,D2=0),1,0)

Copy these conditional tests to all subsequent rows.

Format these columns to zero decimal places; column width is not important, but if these get too wide the subsequent file has the rows spread out over more than one line

- g. In column I set the valid data-point count that omits duplicate and dropped data by placing a "1" in cell I2 and in cell I3 test the flags and adjust the count using $\text{IF}(\text{AND}(\text{G3}=0, \text{H3}=0), \text{I2}+1, \text{I2})$. Copy this conditional calculation to all data points.
- h. Delete any plot sheets, leaving only the data sheet.

After these changes, columns should contain

A	date
B	time
C	B/W RTD Temperature
D	GB RTD Temperature
E	Measured Pressure

- F Excess temperature calculation per the selected algorithm, e.g., Eqn. 8-5.
 - G Duplicate data flag, 0 or 1
 - H Dropped data flag, 0 or 1
 - I Valid data count No., i.e., purged of duplicate or dropped data
4. Save the adjusted-count EXCEL file, in case some modification is needed later, e.g., in a CleanDat\TC-xxx.xls file.
 5. Save a copy of the the adjusted, streaming-data input file as a tab-delimited TEXT file as Stream\STRxxx.TXT for use as input data. When closing, do **not** save this file as an EXCEL format - i.e., hit the “no” button when asked.
 6. Note the number of rows of actual, but raw (not the Valid count) data (i.e., do not include any heading rows).
 7. Note the valid count number for all sample events, calibration events, the reference point, the beta points, etc. (The data input to the advanced versions of the GGE program use the valid point numbers.) Note the measured pressure, RTD temp, GB temp, and T-excess values for these points (these will be used in the SetUp data set, SETxxx.txt, originated as a WP file).
 8. Open the STRxxx.TXT file in WordPerfect (Courier New, 12 pt font), and make the following changes. Note: the resulting file will be directly input to the FORTRAN application program; the changes must be carefully made to have the correct syntax.

Remove labels & headings.

The 1st line will be ignored, so this can be used for identification as desired (suggest “TC-153 Streaming Data Input”). The 2nd line **must** show number of actual (i.e., not including any heading rows) raw, unadjusted data rows, **in format I5**. The 3rd row is ignored and can be used as desired (suggest putting a continuous numbering across the page to facilitate confirmation of proper parameter spacing, step 11, below).

Place tabs **only** at absolute settings of 1, 2, 3, 3-1/2, 4, 5, 5-3/4, 6, & 6-3/8 in. This should give the following columnization:

a.	First 20 characters for date and time	[columns 1-20]
b.	5 characters for each of T _{RTD} and T _{GB}	[columns 21-25 & 26-30]
c.	10 characters for Pressure	[columns 31-40]
d.	7 characters for T-excess	[columns 41-47]
e.	1 character for the duplicate data flag	[column 48]
f.	2 blank spaces	[columns 49-50]
g.	1 character for the dropped data flag	[column 51]

- h. 2 blank spaces [columns 52-53]
 - i. 5 characters for the adjusted data count [columns 54-58]
9. Save the file as a DOS unformatted text file, i.e., just hit the “save” icon.
 10. Confirm the proper parameter spacing by examining this file in DOS using the TYPE {filename}| MORE” command.

Note: further opening of this file in WP will cause it to be in opened in a WPD format — i.e., *space-delimited* form, where previous tabs are obliterated, so further attempts to move columns by manipulating tabs is useless.

Program Use Procedure

The GGE7b1 program uses two input files: GGESET.txt and GGESTR.txt, that are copies of the SETxxx.txt and STRxxx.txt files, respectively.

1. Copy the STRxxx.txt file when ready to use to the file, C:\rmfort\dataset\GGESTR.txt.
2. Copy the SETxxx.txt file when ready to use to the file, C:\rmfort\dataset\GGESET.txt.
3. Execute the desired FORTRAN program version, e.g., GGE7b1.
4. Following the program execution, two output files are created in C:\rmfort\output\:
 - (1) a summary file of approximately 4 Mbytes for 26,000 data points that gives the results based on the valid data point numbers, C:\rmfort\output\GGESUM.out (a space-delimited text file); and
 - (2) a large file of about 48 Mbytes that shows many of the intermediate calculations, primarily for trouble shooting use, C:\rmfort\output\GGE.out.
5. Open the GGESUM.out file into an EXCEL spreadsheet (“fixed-width” type).
6. Delete or move the first 7 rows, which show

VGP	Headspace volume at the Reference Point conditions
TBETA(1)	The low temperature for the BETA-Lo parameter
BETA(1)	BETA-Lo
TBETA(2)	The high temperature for the BETA-Hi parameter
BETA(2)	BETA-Hi
TEXGLB	Ignore this parameter
ICYCLE	Ignore this parameter

7. Adjust the column widths as desired, and label the columns as follows

<u>Column</u>	<u>Label</u>
---------------	--------------

A	Valid Pt. No.
B	Date & Time
C	Measured Pressure
D	Adjusted Pressure
E	HS Gas Mass
F	Vapor Pressure
G	Brine/Waste RTD
H	Glovebox RTD
I	dT-excess
J	Est. Local TC Environment
K	Mole Fraction of Generated Gas Relative to the Value at Ref. Pt. No. {REF}, where {REF} is the number of the point selected as reference and included in the corresponding SETxxx.txt file.

J is calculated as the sum of the Glovebox RTD plus the dT-excess.

K is calculated as (Eqn. 32)

$$\Delta X_{gen} = \frac{P_{adj} - P_0}{P_{adj} - P_{v_{\eta}}}$$

8. Plot the temperatures, pressures, and mole fraction of generated gas columns as line charts.
9. Save this file in Results\TC-xxx as an EXCEL file for later review, if needed.

ATTACHMENT 3 TO APPENDIX D

Program Flow Overview Version - GGE7

MAIN

```

Set subprogram generalities
  Call ONEDIM
  Call VAPOR
  Call CALIBR

Set Reference Point Conditions T' and P', and set parameters
  Call CALIBR ----> corrected T' & P'
  Call ONEDIM----> Tg'
  Call VAPOR----> Pv'
  Call BB-----> set generalities
  Call BB-----> z'
  Call SOLUBL----> set generalities, RNg-dis'

Call SAMPLE----->R*dMs
  >Sample No. just to left & right of Reference Pt.
  >Vs-term (intermediate)
  >R*dMg-sol-s = -R*dMg-dis

DO all samples
  Set sample data
  Call CALIBR----->corrected Ts & Ps
  Call ONEDIM----->Tgs
  Call VAPOR----->Pvs
  Call BB----->Zg-1
  Call BB----->Zg-2
  Call SOLUBL----->R*Ng-dis-s1
  Call SOLUBL----->R*Ng-dis-s2
  Calc Vgs for each sample
  Calc R*dMs
  Establish location of Ref Pt relative to samples

Call BKFILL----->R*dMc
  >Backfill No. just to left & right of Reference Pt.
  >dMc-terms (intermediate)

DO all PXD-calibration backfills
  Set PXD-Calib. data
  Call CALIBR----->corrected Tc & Pc
  Call ONEDIM----->Tgc-1
  Call ONEDIM----->Tgc-2
  Call VAPOR----->Pvc-1
  Call VAPOR----->Pvc-2
  Call BB----->Zgc-1
  Call BB----->Zgc-2
  Call SOLUBL----->Ng-dis-c1
  Call SOLUBL----->Ng-dis-c2
  Calc dMc-term-2 = Pgc-2/Zgc-2/Tgc-2 for use in S/R REFVOL
  Calc dMc-term-1 = Pgc-1/Zgc-1/Tgc-1 for use in S/R REFVOL
  Establish location of Ref. Pt. relative to PXD-calibrations

```

gge\wp\flo-diag-7.wpd

Begin iteration loop to adjust HS volume measurements for commonality at the Reference Pt. conditions and in process determine V_{g-ave} and Beta-Lo and Beta-Hi

Input Beta data, adjusting for calibrations, HS-gas temp and -pressure and compressibility compute

```
DO all Betas
READ Beta-step data
Call CALIBR----->corrected  $T_K$  &  $P_K$ 
Call ONEDIM-----> $T_{gK}$ 
Call VAPOR-----> $P_{vK}$ 
Call BB-----> $Z_K$ 
```

```
READ Beta-start data
Call CALIBR----->corrected  $T_B$  &  $P_B$ 
Call ONEDIM-----> $T_{gB}$ 
Call VAPOR-----> $P_{vB}$ 
Call BB-----> $Z_B$ 
```

DO all samples (V_g measurements)
Set initial guess of V_g at Ref. Pt. Conditions equal to ave of V_{gs}

Begin Iteration Loop for V_{g-ave} at the Ref. Pt. conditions by successive substitution of calculated V_{g-ave} for $V_{g-guess}$

```
Calc  $R \cdot M_g' = P_g \cdot V_{g-guess} / Z' / T_g'$ 
DO all PXD Calibrations
  Calc  $R \cdot dM_c$  using  $dM_c$  terms from S/R BKFILL
  Determine difference in HS-gas mass between Beta-Step and Beta-Start due changes in
  quantity of gas dissolved in brine to find true brine/waste expansion coefficient, Beta
```

```
DO all Beta steps
Call SOLUBL-----> $N_{g-dis-K}$ 
Calc  $R \cdot dM_{g-K}$ 
Call MASRAT-----> $M'/M_K$ 
Call MSUMS ----->Pt location relative to Reference
                        >Sum  $R \cdot dM_g$ 
                        >Sum  $R \cdot dM_c$ 
```

```
Call SOLUBL-----> $N_{g-dis-B}$ 
Calc  $R \cdot dM_{g-B}$ 
Call MASRAT-----> $M'/M_B$ 
Call MSUMS ----->Pt location relative to Reference
                        >Sum  $R \cdot dM_g$ 
                        >Sum  $R \cdot dM_c$ 
```

Calc M_K/M_B

Compute Beta-Lo and Beta-Hi at the ave Beta temperatures

```
DO all samples ( $V_g$  measurements)
Compute adjusted  $V_{gs}$  at the ref temperature
Find the arithmetic ave of all adjusted  $V_{gs}$  (i.e.,  $V_{gs-ave}$ )
Compare  $V_{gs-ave}$  to  $V_{g-guess}$ , iterate as required
```

gge\wp\flo-diag-7.wpd

```

      Calc final value of HS-gas mass at the Ref. Pt.,  $R \cdot dM_g$ 
DO all PXD Calibrations
      Determine HS vol,  $V_{gc-1}$  and  $V_{gc-2}$  at backfill conditions
      Call HSVOL-----> $dV_{gc-1}$ 
          Calc  $dV_c$ 
          Calc Beta-ave (=Beta(T-ave))
          Calc  $V_{gc-1}$  &  $dV_{lc-1}$ 
      Call HSVOL-----> $dV_{gc-2}$ 
          Calc  $dV_c$ 
          Calc Beta-ave (=Beta(T-ave))
          Calc  $V_{gc-2}$  &  $dV_{lc-2}$ 

      Calc  $R \cdot dM_c$  using  $dM_c$  terms-1&-2 from S/R BKFILL

Compute compensated pressure for all data points--input data points
DO all data points
      Adjust data point No. for duplicative or dropped data
      Call CALIBR----->corrected  $T_d$  &  $P_d$ 
      Call ONEDIM-----> $T_{gd}$ 
      Call VAPOR-----> $P_{vd}$ 
      Call BB-----> $Z_d$ 
      Call SOLUBL-----> $R \cdot N_{g-d}$ 
      calc  $R \cdot dM_{g-sol-d}$ 
      Call HSVOL-----> $dV_g$ 
          -----> $V_g$ 
          Calc  $dV_c$ 
          Calc Beta-ave (=Beta(T-ave))
          Calc  $V_{gd}$  &  $dV_{ld}$ 
          compute ratios of ref to data pt for  $z, T, V_g$ 
      Call MASRAT-----> $M'/M$ 
          Call MSUMS ----->Pt location relative to Reference
              >Sum  $R \cdot dM_s$ 
              >Sum  $R \cdot dM_c$ 

      Compute adjusted pressure
END

```

ATTACHMENT 4 TO APPENDIX D

FORTRAN Program GGE7b1 Listing

PROGRAM GGE7b1

```
C
C--ADJUSTMENT TO THE MEASURED PRESSURE WITHIN THE GGE TEST
C  CONTAINERS TO NEGATE EFFECTS OF TEMPERATURE & MASS VARIATION
C
C--AUTHOR: F.S. FELICIONE, ANL-W, TEL. (208) 533-7547
C
C--VERSION 007b IS LIKE VERSION 007a, BUT WITH 5.00 HEADFAC
C  TO ACCOUNT FOR 2-D EFFECTS IN THE HEAD (VERSION 007a USED A
C  FACTOR OF 8.48)- IN S/R XPORT) AND WRITES TEMP BASIS FOR
C  BETA-LO AND BETA-HI TERMS TO THE SUMMARY OUTPUT FILE.  VERSION
C  007b1 INCLUDES TEMPERATURES IN THE OUTPUT FILES FOR PLOTTING
C  USE.
C
      COMMON/MAIN/BETA(5),TBETA(5),DVGC1(20),DVGC2(20),VC,ALPHA
      COMMON/PRIME/TRTDP,VLP,VGP,PGP,TGP,ZP,NPTP
      COMMON/BKFIL/DMCT1(20),DMCT2(20),TRTDC1(20),TRTDC2(20)
1     ,NPTC(20),NCALP,NCLEFT,NCRGHT
      COMMON/SAMP/VGS(20),NPTS(20),NSMPLS,NSLEFT,NSRGHT
1     ,RDMGS,TRTDS(20)
      COMMON/MASS/RDMS(20),RDMC(20),RMGP
      COMMON/VOL/DT,TAVE,DVC,BETBAR,DVL
C
      DIMENSION NPTK(5),PK(5),TRTDK(5),TGBK(5),WBETA(5)
1     ,TEXK(5),NPTB(5),PB(5),TRTDB(5),TGBB(5),TEXB(5)
2     ,TGK(5),PVK(5),PGK(5),ZK(5),TGB(5),PVB(5),PGB(5),ZB(5)
C
      CHARACTER*20 DATEHR
C
C--THIS PROGRAM HAS THE FOLLOWING MAJOR CHARACTERISTICS:
C  (A) USES ONEDIM TO DETERMINE THE TEST CONTAINER HEADSPACE
C       TEMPERATURE (THE ONLY CHANGES MADE TO ONEDIM ARE THOSE
C       NEEDED TO FUNCTION AS A SUBROUTINE RATHER THAN A STAND-
C       ALONE PROGRAM
C  (B) USES THE BEATTIE-BRIDGEMAN EQN OF STATE TO DETERMINE A
C       COMPRESSIBILITY FACTOR (Z) OF FORM  $Z = PV/MRT$ 
C  (C) COMPUTES THE HEADSPACE VOLUME FROM DATA COLLECTED DURING
C       GAS-SAMPLING, CORRECTS THE VOLUME TO THE REFERENCE
C       CONDITIONS, AND COMPUTES THE BEST ESTIMATE (MEAN) FROM
C       THE SEVERAL SAMPLES
C  (D) COMPUTES A THERMAL-EXPANSION COEFFICIENT FOR THE WASTE/
```

```

C      BRINE MIXTURE FROM INDUCED TEMPERATURE STEPS
C      (E) ADJUSTS ALL TEMPERATURE AND PRESSURE DATA FOR ERRORS
C      THAT RESULT FROM CALIBRATION CHECKS

C      (F) TRACKS HS-GAS MASS AS IT CHANGES DUE TO GAS SAMPLE
C      EXTRACTION AND BACKFILL ERRORS DURING PXD CALIBRATION
C      (G) COMPUTES THE MASS OF SOLUBLE HS GAS DISSOLVED IN THE
C      BRINE FOR GIVEN TEMPERATURE AND PRESSURE, AND USES THIS
C      TO COMPUTE THE CHANGES IN HS-GAS MASS AT THE LOCAL
C      CONDITIONS COMPARED TO THAT AT THE REF CONDITIONS
C      (H) USES ALL OF THIS INFORMATION TO COMPENSATE THE MEASURED
C      PRESSURE FOR TEMPERATURE EFFECTS, AND ADJUSTS THE
C      PRESSURE TO THE REFERENCE CONDITIONS
C
C--THE USER PROVIDES INPUT TO THE PROGRAM VIA THE UNFORMATTED
C TEXT FILE GGESET.TXT.  THIS FILE CONTAINS ALL GEOMETRIC INFO,
C MATERIAL PROPERTIES, CERTAIN CONSTANTS, CALIBRATION INFO FOR
C THE RTD'S AND PXD'S, GAS-SAMPLING DATA, REFERENCE CONDITIONS,
C INDUCED TEMPERATURE-STEP DATA, AND (OPTIONALLY) A LIST OF THE
C POINTS TO BE COMPENSATED.  FOR CONVENIENCE, THE USER MAY
C CHOOSE TO PROVIDE THE LIST AS A SEPARATE TEXT FILE, GGESTR.TXT
C VERY USEFUL WHEN THE LIST IS "IMPORTED" TO THIS PROGRAM.
C
C--TWO SPACE-DELIMITED TEXT FILES ARE PRODUCED BY THE PROGRAM:
C      (1) GGE.OUT - THIS FILE WRITES MIRRORS OF VIRTUALLY ALL
C      INPUT TERMS AND INTERMEDIATE COMPUTATION VALUES, MOSTLY
C      FOR USE IN DEBUGGING THE PROGRAM, BUT ALSO TO OBTAIN
C      QUANTITIES SUCH AS TRANSPORT COEFFICIENTS, ETC.
C      (2) GGESUM.OUT - THIS FILE WRITES A VERY FEW KEY PARAMETERS
C      AND THE LIST OF MEASURED AND TEMPERATURE-COMPENSATED
C      PRESSURE.  THIS FILE CAN BE IMPORTED INTO A PLOTTING
C      PROGRAM (SUCH AS EXCEL) FOR GRAPHIC DEPICTION OF RESULTS
C
C      OPEN (UNIT=4,FILE='C:\RMFORT\DATASET\GGESET.TXT',
1  STATUS='OLD', BLANK='ZERO')
C      OPEN (UNIT=9,FILE='C:\RMFORT\OUTPUT\GGESUM.OUT',
1  STATUS='UNKNOWN')
C      OPEN (UNIT=10,FILE='C:\RMFORT\OUTPUT\GGE.OUT',
1  STATUS='UNKNOWN')
C      OPEN (UNIT=3,FILE='C:\RMFORT\DATASET\GGESTR.TXT',
1  STATUS='OLD', BLANK='ZERO')
C
C--ESTABLISH ALL GEOMETRIC FACTORS AND PROPERTIES IN ONEDIM
C      CALL ONEDIM(1,DUM1,DUM2,DUM3,DUM4)
C
C--INPUT VAPOR-PRESSURE DATA INTO S/R VAPOR

```



```

        CALL VAPOR(1,DUM1,DUM2)
C
C--SPECIFY TEST-CONTAINER VOLUME AND LINEAR THERMAL-EXPANSION
C COEFFICIENT
      READ(4,6) VC,ALPHA
      6 FORMAT(/2E10.0)
C
C--SPECIFY THE GLOBAL TEMP EXCESS OF GLOVEBOX INTERIOR RELATIVE
C TO THE MEASUREMENT MADE BY THE GB RTD.
      READ(4,34) TEXGLB
      34 FORMAT(/E10.0)
      WRITE(10,35) TEXGLB
      35 FORMAT('/TEXGLB = ',F5.2)
C
C SPECIFY INITIAL RTD & PRESSURE-XDUCR (PXD) CALIBRATION DATA
C
      CALL CALIBR(1,NDUM1,DUM2,DUM3)
C
C--ESTABLISH OVERALL REFERENCE CONDITIONS (SUFFIX "P") - PRESS,
C RTD TEMP,GB TEMP,(FROM THE DATA RECORDS),EXCESS LOCAL TEMP
C IN GB COMPARED TO WALL MEASUREMENT, AND GLOBAL TEMP EXCESS.
      READ(4,2) NPTP,PP,TRTDP,TGBP,TGBEXP
      2 FORMAT(/I5,5X,4E10.0)
      WRITE(10,15) NPTP
      15 FORMAT('//REFERENCE (PRIME) CONDITIONS: PT. NO.',I7)
C
C--ADJUST RTD TEMPERATURE AND TC PRESSURE PER CALIBRATION DATA
      CALL CALIBR(2,NPTP,TRTDP,PP)
C
C--COMPUTE HS-GAS TEMP FOR REFERENCE CONDITIONS
      CALL ONEDIM(2,TRTDP,TGBP,TGBEXP,TGP)
C
C--DETERMINE VAPOR PRESSURE AT REF CONDITIONS AND SUBTRACT FROM
C TOTAL PRESSURE TO GIVE THE GAS PRESSURE
      CALL VAPOR(2,TGP,PVP)
      PGP=PP-PVP
C
      WRITE(10,3)PP,TRTDP,TGBP,TGBEXP,TGP,PVP
      3 FORMAT('/REFERENCE CONDITIONS: '/5X,'PP [PSIA]',F12.2/5X,
1      'TRTDP [C]',F12.2/5X,'TGBP [C]',F13.2/
2      5X,'TGBEXP [C]',F11.2/5X,'TGP [C]',F14.2/5X,
3      'PVP [PSIA]',F12.3)
C
C--INPUT STATE EQN ONE-TIME PARAMETERS
      CALL BB(1,DUM1,DUM2,DUM3)
C

```

```

C--EVALUATE COMPRESSIBILITY FOR THE REFERENCE STATE
      CALL BB(2,TGP,PGP,ZP)
C
C--SET INITIAL PARAMETERS FOR SOLUBILITY AND DETERMINE THE MOLES
C OF SOLUBLE GAS SPECIE DISSOLVED IN BRINE AT THE REFERENCE
C CONDITIONS (RUNP)
      CALL SOLUBL(1,TRTDP,PGP,RUNP)
C
C--ENTER THE GAS-SAMPLING DATA AND DETERMINE THE HEADSPACE VOLUME
C FROM EACH SAMPLE
      WRITE(10,5)
      5 FORMAT(// 'HS-GAS-SAMPLE-DATA EVALUATION FOR HS VOLUME')
C
      CALL SAMPLE
C
      WRITE(10,43) (I,VGS(I),I=1,NSMPLS)
      43 FORMAT(// 'HS-GAS VOLUME AT THE SAMPLE CONDITIONS - VGS(I)'/
      1 (I3,2X,F10.3))
C
C--USE BACKFILL DATA RECORDED DURING CALIBRATION OF THE PRESSURE
C TRANSDUCERS TO COMPUTE THE HS-MASS INCREASES THAT OCCURRED
C WHEN THE INSTRUMENT DUCT WAS BACKFILLED
C
      CALL BKFILL
C
C--BEGIN AN ITERATION PROCESS TO DETERMINE THE HS-GAS VOLUME AT
C THE REFERENCE CONDITIONS (VGP) FROM THE VOLUMES DEDUCED FROM
C THE MEASUREMENTS BY ADJUSTING THOSE TO COMMON CONDITIONS AT
C THE REFERENCE CONDITIONS. THIS ADJUSTMENT REQUIRES THAT BETA
C BE KNOWN, ITSELF DEPENDENT ON THE HS-GAS VOLUME AT THE REF
C CONDITIONS, SO AN ITERATION IS MADE UNTIL CONVERGENCE WITHIN
C AN ACCEPTABLE RELATIVE RESIDUAL ERROR IS ACHIEVED.
C
C--READ BETA DATA. CONDITIONS AT THE START OF THE BETA STEP HAVE
C A "K" SUFFIX. THE CONDITIONS FOR THE ACTUAL TEMPERATURE STEPS
C HAVE A "B" SUFFIX. CORRECT FOR CALIBRATIONS AND COMPUTE THE
C HS-GAS TEMP, VAPOR PRESSURE, AND COMPRESSIBILITY FACTOR.
      READ(4,8) NBETA
      8 FORMAT(/I5)
      DO 9 I=1,NBETA
      READ(4,29) NPTK(I),PK(I),TRTDK(I),TGBK(I),TEXK(I)
      29 FORMAT(/I5, 5X,4E10.0)
      WRITE(10,28) I
      28 FORMAT(/3X,'* BETA PT. NO.',I5)
C
C--ADJUST RTD TEMPERATURE AND TC PRESSURE PER CALIBRATION DATA

```

```

      CALL CALIBR(2,NPTK(I),TRTDK(I),PK(I))
      CALL ONEDIM(2,TRTDK(I),TGBK(I),TEXK(I),TGK(I))
      CALL VAPOR(2,TGK(I),PVK(I))
      PGK(I)=PK(I)-PVK(I)
      CALL BB(2,TGK(I),PGK(I),ZK(I))
C
      WRITE(10,31)I,PK(I),TRTDK(I),TGBK(I),TEXK(I),TGK(I),PVK(I),
1  ZK(I)
31 FORMAT(/5X,'BETA PT. NO.',I5,' REF. CONDITIONS SUMMARY:'
1  /5X,'PK [PSIA]',F10.2/5X,'TRTDK [C]',F10.2/5X,'TGBK [C]',
2  F11.2/5X,'TEXK [C]',F11.2/5X,'TGK [C]',F12.2/5X,
3  'PVK [PSIA]',F10.3/5X,'ZK',F12.7)
C
      CONTINUE
C
      READ(4,7) NPTB(I),PB(I),TRTDB(I),TGGB(I),TEXB(I)
7  FORMAT(/I5,5X,4E10.0)
C
C--ADJUST RTD TEMPERATURE AND TC PRESSURE PER CALIBRATION DATA
      CALL CALIBR(2,NPTB(I),TRTDB(I),PB(I))
      CALL ONEDIM(2,TRTDB(I),TGGB(I),TEXB(I),TGB(I))
      CALL VAPOR(2,TGB(I),PVB(I))
      PGB(I)=PB(I)-PVB(I)
      CALL BB(2,TGB(I),PGB(I),ZB(I))
C
      WRITE(10,14)I,PB(I),TRTDB(I),TGGB(I),TEXB(I),TGB(I),PVB(I),
1  ZB(I)
14 FORMAT(/5X,'BETA PT. NO.',I5,' SUMMARY:'/5X,
1  'PB [PSIA]',F10.2/5X,'TRTDB [C]',F10.2/5X,'TGGB [C]',
2  F11.2/5X,'TEXB [C]',F11.2/5X,'TGB [C]',F12.2/5X,
3  'PVB [PSIA]',F10.3/5X,'ZB',F12.7)
C
      9 CONTINUE
C
C--BEGIN ACTUAL ITERATION LOOP.  FOR THE 1ST CYCLE GUESS AN
C  INITIAL VALUE FOR THE MEAN HS VOL.  ANY VALUE WILL WORK, AND
C  CONVERGENCE IS VERY RAPID.  FOR SIMPLICITY, USE THE AVE OF THE
C  RAW HS-VOL MEASUREMENTS.  THEN COMPUTE THE IMPLIED PROVISIONAL
C  MEAN BRINE/WASTE VOLUME (VLP)
      SUM=0.
      DO 51 I=1,NSMPLS
      SUM=SUM+VGS(I)
51 CONTINUE
      VGUESS=SUM/NSMPLS
      VLP=VC-VGUESS
C

```

```

WRITE(10,52)VGUESS,VLP
52 FORMAT(/'BEGIN ITERATION FOR MEAN HS VOLUME AND BETA'/
1  'INITIAL ASSUMPTIONS:'/10X,'VGP=',F10.3,10X,'VLP=',F10.3)
C
ICycle=0
ERR=0.00001
MAXCYC=100
C
38 CONTINUE
ICycle=ICycle+1
IF(ICycle .GT. MAXCYC)STOP
1  'MEAN HS VOLUME CYCLE LIMIT REACHED'
C
C--NOW USE SUCCESSIVE SUBSTITUTION TO ITERATE THE AVE HS VOLUME
C AT REF CONDITIONS UNTIL CONVERGED
IF(ICycle .GT. 1)VGUESS=VG0AVE
C
C--THE PRESSURE CHANGE AT THE BETA STEP MAY BE PARTIALLY DUE TO
C A CHANGE IN THE HS-GAS MASS THAT RESULTED FROM A CHANGE IN THE
C QUANTITY OF SOLUBLE GAS DISSOLVED IN THE BRINE. THIS MUST BE
C ACCOUNTED FOR TO YIELD A BETA VALUE THAT REFLECTS ONLY THE
C THE EXPANSION/CONTRACTION CHARACTERISTICS OF THE BRINE/WASTE.
C FOR PROGRAMMING CONVENIENCE, THE RATIO OF HS-GAS MASS BEFORE
C AND AFTER THE BETA STEP ARE FOUND BY COMBINING RATIOS RELATIVE
C TO THE OVERALL REF PT CONDITIONS.
C
C FIRST COMPUTE HS-GAS MASS (*GAS CONSTANT) AT THE REF
C CONDITIONS AND CURRENT ESTIMATE OF HS VOLUME
RMGP=PGP*VGUESS/ZP/(273.15+TGP)
C
DO 58 I=1,NBETA
CALL SOLUBL(2,TRTDK(I),PGK(I),RUNK)
RDMDIS=RUNK-RUNP
RDMGK=-RDMDIS
CALL MASRAT(NPTK(I),RDMGK,WRATK)
C
CALL SOLUBL(2,TRTDB(I),PGB(I),RUNB)
RDMDIS=RUNB-RUNP
RDMGB=-RDMDIS
CALL MASRAT(NPTB(I),RDMGB,WRATB)
C
WBETA(I)=WRATK/WRATB
58 CONTINUE
C
C COMPUTE BETA-LO (BETA(1)) AND BETA-HI (BETA(2)) AT THE AVE
C TEMPERATURES OF THE RESPECTIVE BETA STEPS BASED ON THE CURRENT

```

```

C  VGUESS (NOTE: NBETA=2 ALWAYS, IN THE PRESENT FORMULATION)
    DO 53 I=1,NBETA
      TBETA(I)=(TRTDB(I)+TRTDK(I))/2.
      DTSTEP=TRTDB(I)-TRTDK(I)
      DVC=3.*ALPHA*VC*DTSTEP
      PRATIO=PGK(I)/PGB(I)
      ZRATIO=ZK(I)/ZB(I)
      TRATIO=(TGK(I)+273.15)/(TGB(I)+273.15)
      BRACK=PRATIO*WBETA(I)/ZRATIO/TRATIO-1.
      BRACE=1.+(DVC-VGUESS*BRACK)/VLP
      BETA(I)=1./DTSTEP*ALOG(BRACE)
C
      WRITE(10,12)I,ZRATIO,TRATIO,PRATIO,DTSTEP,TBETA(I),DVC,
1    BRACK,BRACE,BETA(I)
12  FORMAT(/5X,'PARAMETERS FOR BETA PT. NO.',I3
1    /5X,'ZRATIO',F12.7/5X,'TRATIO',F12.7/5X,'PRATIO',
2    F12.7/5X,'DTSTEP',6X,F5.2/5X,'TBETA(I)',4X,F5.2/5X,'DVC',
3    E18.6/5X,'BRACK',E16.6/5X,'BRACE',E16.6/5X,'BETA(I)',
4    E14.6)
C
53  CONTINUE
C
C--NOW COMPUTE THE TEMPERATURE-DEPENDENT VALUE OF BETA (BETAI)
C  APPLICABLE TO EACH VOLUME MEASUREMENT BY LINEARLY
C  INTERPOLATING BETWEEN BETA-LO (IE, BETA(1)) AND BETA-HI
C  (IE, BETA(2)) FROM ABOVE, BASED ON THE AVE TEMPERATURE (TIAVE)
C  BETWEEN THE MEASUREMENTS AND REF RTD TEMPERATURES.
C
C  THEN COMPUTE THE ADJUSTED HS VOLUME FOR EACH MEASUREMENT WHEN
C  ADJUSTED TO THE REF TEMPERATURE (VG0I) AND FIND THE AVE OF
C  THESE (VG0AVE)
      SUM=0.
      DO 54 I=1,NSMPLS
        TIAVE=(TRTDS(I)+TRTDP)/2.
        BBARI=BETA(1)+(BETA(2)-BETA(1))*(TIAVE-TBETA(1))/
1      (TBETA(2)-TBETA(1))
        DTSI=TRTDS(I)-TRTDP
        DVCI=3.*ALPHA*VC*DTSI
        VG0I=(VGS(I)+VC*(EXP(BBARI*DTSI)-1.)-DVCI)/EXP(BBARI*DTSI)
        SUM=SUM+VG0I
54  CONTINUE
      VG0AVE=SUM/NSMPLS
C
C--COMPARE THE CALCULATED AVE HS VOLUME (VG0AVE) TO THE ASSUMED
C  VALUE (VGUESS) AND ITERATE UNTIL THE RELATIVE ERROR IS WITHIN
C  THE USER-SPECIFIED INTERVAL (ERR)

```

```

RELERR=(VG0AVE-VGUESS)/VGUESS
C
WRITE(10,41) ICYCLE,VGUESS,VG0AVE,RELERR,BETA(1),BETA(2)
41 FORMAT(/'MEAN HS VOLUME DETERMINATION CYCLE NO.',I5
1 /10X,'VGUESS=',F10.3/10X,'VG0AVE=',F10.3
2 /10X,'RELERR=',F12.6/10X,'BETA(1)=' ,E15.4
3 /10X,'BETA(2)=' ,E15.4)
IF(ABS(RELERR) .GT. ERR)GO TO 38
C
C--CALCULATE BRINE/WASTE VOLUME AT THE O.A. REFERENCE CONDITIONS
VGP=VG0AVE
VLP=VC-VGP
WRITE(10,11)VGP,VLP
11 FORMAT(/'FINAL REF VALUES'/5X,'VGP',F15.3/5X,'VLP',F14.2)
C
C--COMPUTE FINAL HS-GAS MASS*GAS CONSTANT AT THE REF CONDITIONS
RMGP=PGP*VGP/ZP/(273.15+TGP)
C
C--CALCULATE THE HS VOLUMES AT THE BACKFILL CONDITIONS
DO 57 I=1,NCALP
CALL HSVOL(TRTDC1(I),DVGC1(I),DUM)
CALL HSVOL(TRTDC2(I),DVGC2(I),DUM)
57 CONTINUE
C
C--CALCULATE THE HS-GAS MASS (ACTUALLY GAS CONSTANT*MASS, R*DM)
C INCREASE DURING EACH BACKFILL BASED ON THE ACTUAL HS VOLUME
C AT THE BACKFILL CONDITIONS
DO 55 I=1,NCALP
VC1=VGP+DVGC1(I)
VC2=VGP+DVGC2(I)
RDMC(I)=VC2*DMCT2(I)-VC1*DMCT1(I)
55 CONTINUE
C
WRITE(10,56) RMGP,(I,RDMC(I),I=1,NCALP)
56 FORMAT(/'HS-GAS MASS*R=' ,E15.8/
1 'BACKFILL HS-GAS-MASS INCREASE (R*DMC)'/10X,'I',5X,
2 'RDMC(I)'/ (9X,I2,5X,E12.6))
C
C--GENERATE A SUMMARY FILE OF RESULTS FOR HS-GAS VOLUME, BETA,
C DATA-POINT NO., DATE&HR, MEASURED PRESSURE, FINAL PRESSURE (AS
C ADJUSTED) AND HS-GAS MASS
C
WRITE(9,33) VGP,TBETA(1),BETA(1),TBETA(2),BETA(2),TEXGLB,
1 ICYCLE
33 FORMAT('VGP:',10X,E12.5/'TBETA(1):',7X,E12.4/
1 'BETA(1):',7X,E12.4/'TBETA(2):',7X,E12.4/'BETA(2):',

```

```

      2  7X,E12.4/'TEXGLB:',8X,F5.2/'ICYCLE:',8X,I5/'NDATPT',
      3  5X,'DATE:HR',16X,'PD',8X,'PDADJ',10X,'HS-GAS MASS',
      4  10X,'VAPOR PRESS'/)
C
C
C
C--PERFORM ADJUSTMENTS TO THE MEASURED PRESSURES FOR TEMPERATURE
C  AND HS-GAS-MASS VARIATION
C
C--FOR LATER USE, SPECIFY THE GAS CONSTANT FOR N2 (RN2) IN
C  UNITS OF PSIA-ML/G/K
      RN2=0.08206/28.*14.696*1000.
C
C--SPECIFY WHETHER THE INPUT CONSISTS OF EITHER SELECTED DATA
C  POINTS (ISTRM=0) OR A CONTINUOUS, STREAMING INPUT OF DATA
C  POINTS (ISTRM=1) AND THE NUMBER OF SELECTED DATA POINTS
C  (NDATA) [THIS NDATA VALUE IS USED ONLY IF ISTRM=0]
      READ(4,16) NDATA,ISTRM
      16 FORMAT(/2I5)
C
C--DISCARD HEADER INFO FOR EACH LISTED-INPUT TYPE AND SPECIFY
C  NUMBER OF DATA POINTS IF A STREAMING INPUT LIST IS USED
      IF(ISTRM .EQ. 0)READ(4,26)
      26 FORMAT( )
      IF(ISTRM .EQ. 1)READ(3,40)NDATA
      40 FORMAT(/I5/)
C
C--SPECIFY DATA-POINT CONDITIONS (SUFFIX "D") IN THIS ORDER:
C
C      IF DATA IS NOT STREAMED: PT. NO., DATE&HR,PRESS,RTD
C      TEMP,GB TEMP, LOCAL EXCESS TEMP
C
C      IF DATA IS STREAMED: DATE&HR,RTD TEMP,GB TEMP,PRESS,
C      LOCAL EXCESS TEMP,DUPLICATE DATA FLAG (IDUP),ZERO-DATA
C      (DATA DROPOUT) FLAG (IZERO)
C
      NDATPT=0
      DO 17 I=1,NDATA
      IF(ISTRM .EQ. 1)READ(3,36)DATEHR,TRTDD,TGBD,PD,TEXD,IDUP
      1  ,IZERO
      36 FORMAT(A20,2F5.0,F10.0,F7.0,I1,2X,I1)
C
C--OMIT DATA POINT FROM STREAMING INPUT OPTION IF THIS IS A
C  DUPLICATE OR INVOLVES DROPPED DATA (IE IF IDUP=1 OR IZERO=1).
C  THE LOOP COUNT PERTAINS TO THE EXCEL RAW NUMBERING, BUT ONLY
C  POINTS THAT ARE NOT DUPLICATED OR DROPPED (ZERO) ARE ADJUSTED.

```

```

C THE EXCEL RAW DATA POINT NO. IS PRESERVED IN THE OUTPUT FILE,
C BUT ALL SAMPLES, CALIBRATIONS, REFERENCE POINTS, BETA POINTS,
C ETC REFER TO THE POINT NO. WHEN ADJUSTED FOR DUPLICATE AND
C DROPPED (ZERO) DATA.
C
      IF(ISTRM .EQ. 1 .AND. IDUP .EQ. 1)GO TO 17
      IF(ISTRM .EQ. 1 .AND. IZERO .EQ. 1)GO TO 17
      NDATPT=NDATPT+1
      IF(ISTRM .EQ. 0)READ(4,18)NDATPT,DATEHR,PD,TRTDD,TGBD,TEXD
18  FORMAT(I5,A20,4E10.0)
C
C--DETERMINE THE DATA POINT HS-GAS TEMP, VAPOR PRESS, AND
C COMPRESSIBILITY FACTOR BY CALLING S/R ONEDIM, S/R VAPOR, AND
C S/R BB, AS WAS DONE FOR THE OTHER POINTS ABOVE.
C EVALUATE BETA AT THE AVERAGE TEMP BETWEEN REF AND DATA.
C THEN DETERMINE THE TEST-CONTAINER EXPANSION AND THE
C WASTE/BRINE EXPANSION RELATIVE TO THE REFERENCE CONDITIONS.
C FINALLY, COMPUTE THE REF/DATA RATIOS FOR Z, TG, AND VG. THE
C TEMP-ADJUSTED PRESSURE IS PGD*ZRATIO*TRATIO/VRATIO*WRATIO.
C
C--THE CURRENT CONSTRUCT ASSUMES TWO BETA VALUES ONLY: BETA(1),
C A LOW-TEMP STEP VALUE AT TEMP TBETA(1) AND BETA(2), A HIGH-
C TEMP STEP VALUE AT TEMP TBETA(2). THE BETA VALUE FOR USE IN
C THE PRESS ADJUSTMENT IS BETBAR (BETA-BAR, IE AVE) DETERMINED
C BY INTERPOLATING LINEARLY BETWEEN BETA(1) AND BETA(2) AT THE
C AVE TC RTD TEMP.
C
      WRITE(10,19) NDATPT,DATEHR,PD,TRTDD,TGBD,TEXD
19  FORMAT(/'*****'
1    /'***NEW DATA POINT*****'
2    /5X,'NDATPT',I9/5X,'DATE:HR',A20/5X,'PD',F13.2/5X,
3    'TRTDD',F10.2/5X,'TGBD',F11.2/5X,'TEXD',F11.2)
C
C--ADJUST RTD TEMPERATURE PER CALIBRATION DATA
      CALL CALIBR(2,NDATPT,TRTDD,PD)
C
      CALL ONEDIM(2,TRTDD,TGBD,TEXD,TGD)
      CALL VAPOR(2,TGD,PVD)
      WRITE(10,27) TGD
27  FORMAT(/5X,'HS-GAS TEMP, TGD, FROM ONEDIM:',F8.3)
      PGD=PD-PVD
      CALL BB(2,TGD,PGD,ZD)
C
C--DETERMINE THE MOLES OF SOLUBLE GAS SPECIE DISSOLVED IN BRINE
C AT THE DATA-POINT CONDITIONS TIMES UNIV GAS CONSTANT (RUND)
      CALL SOLUBL(2,TRTDD,PGD,RUND)

```



```

RDMDIS=RUND-RUNP
RDMGD= -RDMDIS
C
C--CALCULATE HS-GAS VOLUME AT THE DATA-POINT CONDITIONS
CALL HSVOL(TRTDD,DVG,VGD)
C
C--FORM RATIOS TO THE REFERENCE STATE
ZRATIO=ZP/ZD
TRATIO=(273.15+TGP)/(273.15+TGD)
VRATIO=VGP/VGD
CALL MASRAT(NDATPT,RDMGD,WRATIO)
C
C--CALCULATE THE HS-GAS MASS AT THIS POINT (ASSUMED PURE N2 GAS)
RMG=RMGP/WRATIO
GMASS=RMG/RN2
C
WRITE(10,22) PVD,PGD,DT,TAVE,DVC,BETBAR,DVL,DVG,VGD
22 FORMAT(/5X,'VARIOUS TERMS'/5X,'PVD',F8.3/5X,'PGD',F8.2
1 /5X,'DT',F8.3/5X,'TAVE',F8.3/5X,'DVC',E12.4
2 /5X,'BETBAR',E12.4/5X,'DVL',F8.3/5X,'DVG',F8.3
3 /5X,'VGD',F8.3)
WRITE(10,23) ZRATIO,TRATIO,VRATIO,WRATIO
23 FORMAT(/5X,'RATIOS ZP/ZD, TGP/TGD, VGD/VGP, MD/MP (WRATIO) '
1 /5X,'ZRATIO',F12.7/5X,'TRATIO',F12.7/5X,'VRATIO',F12.7
2 /5X,'WRATIO',F12.7)
C
C--FINALLY, COMPENSATE THE PRESSURE USING THE RATIOS ABOVE
PGDADJ=PGD*ZRATIO*TRATIO/VRATIO*WRATIO
PDADJ=PGDADJ+PVP
WRITE(10,24) NDATPT,DATEHR,PGDADJ,PDADJ
24 FORMAT(/5X,'ADJUSTED PRESSURE: PT. NO.',I7,5X,A20
1 /5X,'PGDADJ',F10.2/5X,'PDADJ',F10.2)
C
WRITE(9,32) NDATPT,DATEHR,PD,PDADJ,GMASS,PVD,TRTDD,TGBD,
1 TEXTD
32 FORMAT(I7,5X,A20,7(5X,F10.2))
17 CONTINUE
C
WRITE(9,50) NDATA
50 FORMAT(/'NDATA=',I10)
STOP
END
C-----
-
C-----
-

```

```

SUBROUTINE HSVOL(TL,DVG,VG)
C
COMMON/MAIN/BETA(5),TBETA(5),DVGC1(20),DVGC2(20),VC,ALPHA
COMMON/PRIME/TRTDP,VLP,VGP,PGP,TGP,ZP,NPTP
COMMON/BKFIL/DMCT1(20),DMCT2(20),TRTDC1(20),TRTDC2(20)
1  ,NPTC(20),NCALP,NCLEFT,NCRGHT
COMMON/SAMP/VGS(20),NPTS(20),NSMPLS,NSLEFT,NSRGHT
1  ,RDMGS,TRTDS(20)
COMMON/MASS/RDMS(20),RDMC(20),RMGP
COMMON/VOL/DT,TAVE,DVC,BETBAR,DVL
C
C--THIS SUBROUTINE DETERMINES THE HS-GAS VOLUME AT THE CURRENT
C CONDITIONS FROM THE TEST-CONTAINER VOLUME, ITS THERMAL
C EXPANSION, AND THE LIQUID/WASTE THERMAL EXPANSION.
DT=TL-TRTDP
TAVE=(TL+TRTDP)/2.
DVC=3.*ALPHA*VC*DT
C
BETBAR=BETA(1)+(BETA(2)-BETA(1))*(TAVE-TBETA(1))/
1 (TBETA(2)-TBETA(1))
WRITE(10,2)BETBAR,BETA(1),BETA(2),TBETA(1),TBETA(2)
2 FORMAT(/'BETBAR=',E15.5,2X,'BETA(1)=',E15.5,2X,'BETA(2)='
1 ,E15.5,2X,'TBETA(1)=',E15.5,2X,'TBETA(2)=',E15.5)
DVL=VLP*(EXP(BETBAR*DT)-1.)
DVG=DVC-DVL
VG=VGP+DVG
C
RETURN
END
C-----
-
C-----
-
SUBROUTINE SAMPLE
C
COMMON/MAIN/BETA(5),TBETA(5),DVGC1(20),DVGC2(20),VC,ALPHA
COMMON/PRIME/TRTDP,VLP,VGP,PGP,TGP,ZP,NPTP
COMMON/BKFIL/DMCT1(20),DMCT2(20),TRTDC1(20),TRTDC2(20)
1  ,NPTC(20),NCALP,NCLEFT,NCRGHT
COMMON/SAMP/VGS(20),NPTS(20),NSMPLS,NSLEFT,NSRGHT
1  ,RDMGS,TRTDS(20)
COMMON/MASS/RDMS(20),RDMC(20),RMGP
COMMON/VOL/DT,TAVE,DVC,BETBAR,DVL
C
DIMENSION PGS1(20),PGS2(20),ZS1(20),ZS2(20),TGS(20)
C

```

```

C--THIS SUBROUTINE TREATS THE DATA GATHERED DURING SAMPLING OF
C THE HS GAS. THE HS VOLUME (AT THE SAMPLE CONDITIONS) IS
C DEDUCED, THE MASS OF GAS EXTRACTED IS DETERMINED, AND THE
C CHRONOLOGY OF SAMPLES RELATIVE TO THE USER-SELECTED REFERENCE
C POINT IS DETERMINED
C
C--INPUT SAMPLE MEASUREMENTS: SAMPLE VOLUME IS VSAMPL; THE NUMBER
C OF SAMPLE POINTS IS NSMPLS
      READ(4,1)VSAMPL
      1 FORMAT(/E10.0)
      READ(4,4)NSMPLS
      4 FORMAT(/I5)
      IF(NSMPLS .EQ. 0)STOP'NO HS-GAS SAMPLE INPUT PROVIDED'
C
C--INPUT GAS-SAMPLE DATA AND COMPUTE PARAMETERS FOR EACH OF THE
C NSMPLS TOTAL SAMPLE PTS
      READ(4,11)
      11 FORMAT( )
C
      DO 3 I=1,NSMPLS
      WRITE(10,15) I
      15 FORMAT(/'SAMPLE NO.',I4,' POINT EVALUATION')
      READ(4,2) NPTS(I),PS1,PS2,TRTDS(I),TGBS,TGBEXS
      2 FORMAT(3X,1X,I5,1X,5E10.0)
C
C--ADJUST RTD TEMPERATURE & TC PRESSURE PER CALIBRATION DATA
C (PS1 & PS2 ARE ADJUSTED SIMULTANEOUSLY)
      PS=PS1
      CALL CALIBR(2,NPTS(I),TRTDS(I),PS)
      ADJ=PS-PS1
      PS1=PS1+ADJ
      PS2=PS2+ADJ
C
C--COMPUTE THE HEADSPACE GAS TEMPERATURE FOR THIS SAMPLE DATA
      CALL ONEDIM(2,TRTDS(I),TGBS,TGBEXS,TGS(I))
C
C--DETERMINE WATER VAPOR PRESSURE FOR THIS SAMPLE DATA AND
C SUBTRACT FROM THE TOTAL PRESSURE TO GIVE SAMPLE GAS PRESSURE
      CALL VAPOR(2,TGS(I),PVS)
      PGS1(I)=PS1-PVS
      PGS2(I)=PS2-PVS
C
C--DETERMINE THE COMPRESSIBILITY FACTORS ZS1 & ZS2
      CALL BB(2,TGS(I),PGS1(I),ZS1(I))
      CALL BB(2,TGS(I),PGS2(I),ZS2(I))
C

```

```

C--DETERMINE THE MOLES OF SOLUBLE GAS SPECIE DISSOLVED IN BRINE
C  FOR THESE SAMPLE CONDITIONS (RUNS1 AND RUNS2) AND THE CHANGES
C  IN HS GAS MASS TIMES R (RDMGS)
      CALL SOLUBL(2,TRTDS(I),PGS1(I),RUNS1)
      CALL SOLUBL(2,TRTDS(I),PGS2(I),RUNS2)
      RDMDIS=RUNS2-RUNS1
      RDMGS= -RDMDIS
C
C--CALCULATE THE HEADSPACE-GAS VOLUME FOR THIS MEASUREMENT
      TRM1=PGS1(I)/ZS1(I)
      TRM2=PGS2(I)/ZS2(I)
      VGS(I)=(TRM2*VSAMPL-RDMGS*(TGS(I)+273.15))/(TRM1-TRM2)
C
C--CALCULATE THE HS-GAS MASS (ACTUALLY GAS CONSTANT*MASS, R*DMS)
C  ADDED (NEGATIVE OF AMT. EXTRACTED) DURING THIS GAS SAMPLE
      RDMS(I)=-TRM2*VSAMPL/(273.15+TGS(I))
C
      WRITE(10,6) I,TGS(I),PVS,ZS1(I),ZS2(I),VGS(I),RDMS(I)
6  FORMAT(/5X,'SAMPLE NO.',I3,1X,'SUMMARY'/10X,'TGS =',F6.2/
1  10X,'PVS =',F7.3/10X,'ZS1 =',F10.7/10X,'ZS2 =',F10.7/
2  10X,'VGS =',F8.2/10X,'RDMS =',E12.6)
C
3  CONTINUE
C
      WRITE(10,7)(I,RDMS(I),I=1,NSMPLS)
7  FORMAT(/'SAMPLE MASS EXTRACTION (R*DMS)'/
1  10X,'I',5X,'RDMS(I)'/ (9X,I2,5X,E12.6))
C
C--DETERMINE THE NUMBER OF THE LAST SAMPLE POINT (NSLEFT) JUST
C  PRIOR TO (IE,TO THE LEFT OF) THE O.A. REFERENCE POINT; NSRGHT
C  IS THE FIRST SAMPLE POINT AFTER (IE TO THE RIGHT OF) THE O.A.
C  REF POINT
      DO 44 I=1,NSMPLS
      NSLEFT=I
      IF(NPTS(I) .GE. NPTP)GO TO 45
44  CONTINUE
      GO TO 50
45  NSLEFT=I-1
50  CONTINUE
      NSRGHT=NSLEFT+1
      WRITE(10,20)NSLEFT,NSRGHT
20  FORMAT(/5X,'NSLEFT = ',I3,5X,'NSRGHT = ',I3)
C
      RETURN
      END

```

```

C-----
-
C-----
-
      SUBROUTINE BKFILL
C
      COMMON/MAIN/BETA(5),TBETA(5),DVGC1(20),DVGC2(20),VC,ALPHA
      COMMON/PRIME/TRTDP,VLP,VGP,PGP,TGP,ZP,NPTP
      COMMON/BKFIL/DMCT1(20),DMCT2(20),TRTDC1(20),TRTDC2(20)
1      ,NPTC(20),NCALP,NCLEFT,NCRGHT
      COMMON/SAMP/VGS(20),NPTS(20),NSMPLS,NSLEFT,NSRGHT
1      ,RDMGS,TRTDS(20)
      COMMON/MASS/RDMS(20),RDMC(20),RMGP
      COMMON/VOL/DT,TAVE,DVC,BETBAR,DVL
C
      DIMENSION TGC1(20),TGC2(20),PGC1(20),PGC2(20),ZC1(20)
1      ,ZC2(20)
C
C--THIS SUBROUTINE DETERMINES THE HS-MASS CHANGE BY ERROR IN THE
C BACKFILL AND LOCATES THE CHRONOLOGY OF THE PXD CALIBRATIONS
C RELATIVE TO THE REFERENCE POINT
C
C--SPECIFY BACKFILL DATA ASSOCIATED WITH EACH PRESSURE TRANSDUCER
C CALIBRATION
      READ(4,28)
28  FORMAT( )
      DO 30 I=1,NCALP
      WRITE(10,31) I
31  FORMAT(/'PXD CALIBRATION NO.',I4,' POINT EVALUATION')
      READ(4,29) NPTC(I),PC1,PC2,TRTDC1(I),TRTDC2(I),TGBC,TGBEXC
29  FORMAT(3X,I6,1X,5F10.0,F5.0)
C
C--ADJUST RTD TEMPERATURE & TC PRESSURE FOR THIS POINT PER
C CALIBRATION DATA (TC1 & TC2 AND PC1 & PC2 ARE ADJUSTED
C SIMULTANEOUSLY)
      TC=TRTDC1(I)
      PC=PC1
      CALL CALIBR(2,NPTC(I),TC,PC)
      ADJ=PC-PC1
      PC1=PC1+ADJ
      PC2=PC2+ADJ
      ADJ=TC-TRTDC1(I)
      TRTDC1(I)=TRTDC1(I)+ADJ
      TRTDC2(I)=TRTDC2(I)+ADJ
C
C--COMPUTE THE HEADSPACE GAS TEMPERATURE FOR THIS CALIBRATION

```

```

C  DATA
      CALL ONEDIM(2,TRTDC1(I),TGBC,TGBEXC,TGC1(I))
      CALL ONEDIM(2,TRTDC2(I),TGBC,TGBEXC,TGC2(I))
C
C--DETERMINE WATER VAPOR PRESSURE FOR THIS CALIBRATION DATA AND
C  SUBTRACT FROM THE TOTAL PRESSURE TO GIVE SAMPLE GAS PRESSURE
      CALL VAPOR(2,TGC1(I),PVC)
      PGC1(I)=PC1-PVC
      CALL VAPOR(2,TGC2(I),PVC)
      PGC2(I)=PC2-PVC
C
C--DETERMINE THE COMPRESSIBILITY FACTORS ZC1 & ZC2
      CALL BB(2,TGC1(I),PGC1(I),ZC1(I))
      CALL BB(2,TGC2(I),PGC2(I),ZC2(I))
C
C--DETERMINE THE MOLES OF SOLUBLE GAS SPECIE DISSOLVED IN BRINE
C  AT THESE BACKFILL CONDITIONS (ANC1 & ANC2)
      CALL SOLUBL(2,TRTDC1,PGC1(I),ANC1)
      CALL SOLUBL(2,TRTDC2,PGC1(I),ANC1)
C
      WRITE(10,32) I,TGC1(I),TGC2(I),PVC,ZC1(I),ZC2(I)
32  FORMAT(/5X,'PXD CAL NO.',I3,1X,'SUMMARY'/10X,'TGC1 =',F6.2
1    ,10X,'TGC2=',F6.2/10X,'PVC =',F7.3/10X,'ZC1 =',F10.7/
2    10X,'ZC2 =',F10.7)
C
C--SAVE THE R*DMC/VOL TERM FOR USE IN S/R REFVOL
      DMCT2(I)=PGC2(I)/ZC2(I)/(273.15+TGC2(I))
      DMCT1(I)=PGC1(I)/ZC1(I)/(273.15+TGC1(I))
C
30  CONTINUE
C
C--DETERMINE THE NUMBER OF THE LAST PRESSURE TRANSDUCER
C  CALIBRATION POINT (NCLEFT) JUST PRIOR TO (IE, TO THE LEFT OF)
C  THE O.A. REFERENCE POINT; NCRGHT IS THE FIRST CALIBRATION
C  POINT AFTER (IE TO THE RIGHT OF) THE O.A. REF POINT
      DO 22 I=1,NCALP
      NCLEFT=I
      IF(NPTC(I) .GE. NPTP)GO TO 21
22  CONTINUE
      GO TO 23
21  NCLEFT=I-1
23  CONTINUE
      NCRGHT=NCLEFT+1
      WRITE(10,24) NCLEFT,NCRGHT
24  FORMAT(/5X,'NCLEFT = ',I3,5X,'NCRGHT = ',I3)
C

```

```

      RETURN
      END
C-----
-
C-----
-
      SUBROUTINE MASRAT(NPT,RDMX,WRATIO)
C
      COMMON/MAIN/BETA(5),TBETA(5),DVGC1(20),DVGC2(20),VC,ALPHA
      COMMON/PRIME/TRTDP,VLP,VGP,PGP,TGP,ZP,NPTP
      COMMON/BKFIL/DMCT1(20),DMCT2(20),TRTDC1(20),TRTDC2(20)
1    ,NPTC(20),NCALP,NCLEFT,NCRGHT
      COMMON/SAMP/VGS(20),NPTS(20),NSMPLS,NSLEFT,NSRGHT
1    ,RDMGS,TRTDS(20)
      COMMON/MASS/RDMS(20),RDMC(20),RMGP
      COMMON/VOL/DT,TAVE,DVC,BETBAR,DVL
C
C--THIS SUBROUTINE DETERMINES THE RATIO OF THE HS-GAS MASS
C AT THE REFERENCE POINT TO THE HS-GAS MASS AT THE POINT UNDER
C CONSIDERATION (THE VARIATION IS DUE TO SAMPLING AND BACKFILLS)
      CALL MSUMS(NPT,SUMS,SUMC,NPTLOC)
      GO TO (10,20,30),NPTLOC
C
10  CONTINUE
C
C--POINT IS PRIOR TO REFERENCE POINT
      WRATIO=RMGP/(RMGP-SUMS-SUMC+RDMX)
      GO TO 11
C
20  CONTINUE
C
C--POINT COINCIDES WITH THE REFERENCE POINT
      WRATIO=1.0
      GO TO 11
C
30  CONTINUE
C
C--POINT IS PAST THE REFERENCE POINT
      WRATIO=RMGP/(RMGP+SUMS+SUMC+RDMX)
C
11  CONTINUE
      WRITE(10,12)NPT,SUMS,SUMC,RDMX,WRATIO
12  FORMAT(/5X,'MASRAT CALCULATIONS:'/5X,'NPT=',I8/5X,'SUMS=',
1    E15.5/5X,'SUMC=',E15.5/5X,'RDMX=',E15.5/5X,'WRATIO=',
2    E15.5)
C

```

```

        RETURN
        END
C-----
-
C-----
-
        SUBROUTINE MSUMS(NPT,SUMS,SUMC,NPTLOC)
C
        COMMON/MAIN/BETA(5),TBETA(5),DVGC1(20),DVGC2(20),VC,ALPHA
        COMMON/PRIME/TRTDP,VLP,VGP,PGP,TGP,ZP,NPTP
        COMMON/BKFIL/DMCT1(20),DMCT2(20),TRTDC1(20),TRTDC2(20)
1      ,NPTC(20),NCALP,NCLEFT,NCRGHT
        COMMON/SAMP/VGS(20),NPTS(20),NSMPLS,NSLEFT,NSRGHT
1      ,RDMGS,TRTDS(20)
        COMMON/MASS/RDMS(20),RDMC(20),RMGP
        COMMON/VOL/DT,TAVE,DVC,BETBAR,DVL
C
C--THIS S/R LOCATES THE POINT RELATIVE TO THE HS-GAS SAMPLE
C AND PRESSURE-TRANSDUCER-CALIBRATION POINTS, AND SUMS THE
C HS-GAS MASS DIFFERENCES BETWEEN THE POINT UNDER CONSIDERATION
C (NPT) AND THE REFERENCE POINT (NPTP) FROM SAMPLING AND PXD
C CALIBRATIONS
C
C      WRITE(10,26) NPTP
26  FORMAT(/'NPTP=',I5)
C      WRITE(10,9)NSMPLS,NSLEFT,NSRGHT,NCALP,NCLEFT,NCRGHT
9   FORMAT(/'SAMPLES ',3I8/'CALIBRATIONS ',3I8)
C      WRITE(10,12) (N,NPTS(N),N=1,NSMPLS)
12  FORMAT(/'N, NPTS(N) '/(5X,I3,2X,I6))
C      WRITE(10,27) (N,NPTC(N),N=1,NCALP)
27  FORMAT(/'N, NPTC(N) '/(5X,I3,2X,I6))
C
C--DETERMINE LOCATION OF POINT RELATIVE TO THE REFERENCE
      IF(NPT - NPTP)100,200,300
C
100  CONTINUE
      NPTLOC=1
C
C--POINT IS PRIOR IN TIME TO THE REFERENCE POINT
C
C CHECK PT. LOCATION RELATIVE TO SAMPLES. DETERMINE THE SAMPLE
C NO. JUST TO THE RIGHT OF THE POINT
      IF(NSLEFT .EQ. 0)GO TO 19
      DO 4 N=1,NSLEFT
      IF(NPT .LE. NPTS(N))GO TO 5
4    CONTINUE

```



```

19 SUMS=0.
   GO TO 15
C
   5 SUMS=0.
     DO 13 I=N,NSLEFT
       SUMS=SUMS+RDMS(I)
13 CONTINUE
C
15 CONTINUE
C
C--SIMILARLY, CHECK PT. LOCATION RELATIVE TO PXD CALIBRATIONS
C DETERMINE THE CALIBRATION NO. JUST TO THE RIGHT OF THE POINT
   IF(NCLEFT .EQ. 0)GO TO 14
   DO 16 N=1,NCLEFT
     IF(NPT .LE. NPTC(N))GO TO 17
16 CONTINUE
14 SUMC=0.
   RETURN
C
17 SUMC=0.
   DO 18 I=N,NCLEFT
     SUMC=SUMC+RDMC(I)
18 CONTINUE
   RETURN
C
C
300 CONTINUE
   NPTLOC=3
C
C--POINT IS BEYOND THE REFERENCE POINT IN TIME
C
C--CHECK PT. LOCATION RELATIVE TO SAMPLES   DETERMINE THE NO. OF
C THE LAST SAMPLE BEFORE THE POINT.
   IF(NSRGHT .GT. NSMPLS)GO TO 7
C
   DO 6 N=NSRGHT,NSMPLS
     NBK=NSMPLS+NSRGHT-N
     IF(NPT .GT. NPTS(NBK))GO TO 8
6 CONTINUE
C
7 CONTINUE
   SUMS=0.
   GO TO 22
C
8 SUMS=0.
   DO 20 I=NSRGHT,NBK

```

```

        SUMS=SUMS+RDMS( I )
20  CONTINUE
C
22  CONTINUE
C
C--SIMILARLY, CHECK PT. LOCATION RELATIVE TO THE PXD CALIBRATIONS
C  DETERMINE THE NO. OF THE LAST CALIBRATION BEFORE THIS POINT.
        IF(NCRGHT .GT. NCALP)GO TO 21
C
        DO 24 N=NCRGHT,NCALP
        NBK=NCALP+NCRGHT-N
        IF(NPT .GT. NPTC(NBK))GO TO 25
24  CONTINUE
C
21  CONTINUE
        SUMC=0.
        RETURN
C
25  SUMC=0.
        DO 28 I=NCRGHT,NBK
        SUMC=SUMC+RDMC( I )
28  CONTINUE
        RETURN
C
200 CONTINUE
        NPTLOC=2
C
C--POINT IS CO-LOCATED WITH THE REFERENCE POINT
        SUMS=0.
        SUMC=0.
        RETURN
C
        END
C-----
-
C-----
-
        SUBROUTINE CALIBR( ISTRT,NPT,TRUT,TRUP )
C
        COMMON/MAIN/BETA( 5 ),TBETA( 5 ),DVGC1( 20 ),DVGC2( 20 ),VC,ALPHA
        COMMON/PRIME/TRTDP,VLP,VGP,PGP,TGP,ZP,NPTP
        COMMON/BKFIL/DMCT1( 20 ),DMCT2( 20 ),TRTDC1( 20 ),TRTDC2( 20 )
1   ,NPTC( 20 ),NCALP,NCLEFT,NCRGHT
        COMMON/SAMP/VGS( 20 ),NPTS( 20 ),NSMPLS,NSLEFT,NSRGHT
1   ,RDMGS,TRTDS( 20 )
        COMMON/MASS/RDMS( 20 ),RDMC( 20 ),RMGP

```

```

COMMON/VOL/DT,TAVE,DVC,BETBAR,DVL
C
      DIMENSION COMPT(20),COMPP(20),RESIDT(20),RESIDP(20),
1    NCLPTT(20),NCLPTP(20)
C
C--THIS SUBROUTINE TREATS THE CALIBRATION COMPENSATIONS MADE TO
C BOTH THE RTD (T) AND THE PRESSURE XDUCR (P)
C
      GO TO (221,222),ISTRT
221 CONTINUE
C
C--SPECIFY NUMBER OF RTD CALIBRATIONS, THE POINT NO. JUST PRIOR
C TO THE CALIBRATIONS AND THE COMPENSATIONS (INCREASES) MADE TO
C THE DAS AND THE RESIDUAL ERRORS FOR BOTH RTD AND PRESSURE
C XDUCR, AS RECORDED IN THE TC LOG BOOK
      READ(4,1) NCALT,NCALP
1    FORMAT(/2I5)
      READ(4,2)
2    FORMAT( )
      READ (4,3) (NCLPTT(I),COMPT(I),RESIDT(I),I=1,NCALT)
3    FORMAT(15X,I5,5X,2E10.0)
      READ (4,8)
8    FORMAT( )
      READ (4,9) (NCLPTP(I),COMPP(I),RESIDP(I),I=1,NCALP)
9    FORMAT(15X,I5,5X,2E10.0)
C
C--SAVE DATA-POINT DATA FOR THE PRESSURE CALIBRATIONS UNDER A
C DIFFERENT NAME FOR COMMONALITY OF TERMINOLOGY IN ANOTHER S/R
      DO 16 I=1,NCALP
      NPTC(I)=NCLPTP(I)
16 CONTINUE
C
      RETURN
C
222 CONTINUE
C
C--DETERMINE THE TRUE RTD TEMPERATURE TC PRESSURE BY ADJUSTING
C THE RECORDED VALUES WITH THE CALIBRATION DATA. A LINEAR
C DEGRADATION BETWEEN CALIBRATION PTS IS ASSUMED. THE METHOD
C ACCOUNTS FOR RESIDUAL ERRORS REMAINING AFTER THE COMPENSATION
C (COMPT OR COMPP) IS MADE. BOTH COMPENSATION AND RESIDUAL
C ERRORS ARE POSITIVE WHEN THE MEASURED VALUE IS LOW RELATIVE TO
C THE STANDARD
C
C--IDENTIFY THE APPLICABLE CALIBRATION INTERVAL FOR THE
C DATA POINT, THEN ESTIMATE THE TRUE RTD TEMPERATURE (TRUT)

```

```

      DO 4 I=1,NCALT
      IF(NPT .LE. NCLPTT(I))GO TO 5
4  CONTINUE
      ADJMT=0.
      GO TO 6
5  DIFF=NPT-NCLPTT(I-1)
      DUR=NCLPTT(I)-NCLPTT(I-1)
      FRACT=DIFF/DUR
      ADJMT=FRACT*(COMPT(I)+RESIDT(I))+RESIDT(I-1)*(1.-FRACT)
6  TRUT=TRUT+ADJMT
      WRITE(10,7) TRUT,ADJMT
7  FORMAT(/5X,'RTD TRUE TEMP =',F8.3,5X,'TOTAL ADJMT =',F8.3)
C
C--REPEAT THE ADJUSTMENT PROCESS FOR THE PRESSURE XDUCR
C  CALIBRATION
      DO 10 I=1,NCALP
      IF(NPT .LE. NCLPTP(I))GO TO 11
10  CONTINUE
      ADJMT=0.
      GO TO 12
11  DIFF=NPT-NCLPTP(I-1)
      DUR=NCLPTP(I)-NCLPTP(I-1)
      FRACT=DIFF/DUR
      ADJMT=FRACT*(COMPP(I)+RESIDP(I))+RESIDP(I-1)*(1.-FRACT)
12  TRUP=TRUP+ADJMT
      WRITE(10,13) TRUP,ADJMT
13  FORMAT(/5X,'TRUE TC PRESS =',F8.3,5X,'TOTAL ADJMT =',F8.3)
C
      RETURN
      END
C-----
-
C-----
-
      SUBROUTINE VAPOR(ISTRT,TG,PV)
C
      DIMENSION T(100),P(100)
C
C--THIS SUBROUTINE INTERPOLATES A TABLE OF VAPOR PRESSURES TO
C  FIND THE VALUE FOR A SPECIFIED TEMPERATURE
      GO TO (21,22),ISTRT
C
21  CONTINUE
      READ(4,1)NTABL
1  FORMAT(/I5)
      READ(4,4)(T(I),P(I),I=1,NTABL)

```

```

      4 FORMAT(10X,2E10.0)
      RETURN
C
C--LINEARLY INTERPOLATE VAPOR-PRESSURE TABLE
      22 CONTINUE
          DO 2 I=1,NTABL
              IF(TG .GT. T(I))GO TO 2
              PV=P(I-1)+(P(I)-P(I-1))*(TG-T(I-1))/(T(I)-T(I-1))
C
C--CONVERT FROM BAR TO PSIA
          PV=PV*14.5038
          GO TO 3
      2 CONTINUE
          STOP 'VAPOR-PRESSURE TABLE INSUFFICIENT'
C
      3 CONTINUE
C
      RETURN
      END
C-----
-
C-----
-
      SUBROUTINE SOLUBL(ISTRT,TB,PG,RUNDIS)
C
C--THIS SUBROUTINE CALCULATES THE QUANTITY OF THE PRIMARY HS GAS
C (NITROGEN) THAT IS DISSOLVED IN THE LIQUID (BRINE) AT THE
C GIVEN CONDITIONS. THE USER SPECIFIES THE BRINE TEMPERATURE
C (TB), THE SOLUBLE-GAS HS PRESSURE (PG), AND THE SOLUBILITY
C CONSTANTS; THE NUMBER OF MOLES OF GAS DISSOLVED (ACTUALLY
C UNIV GAS CONSTANT * MOLES (RUNDIS)) IS CALCULATED AND
C RETURNED.
C
      GO TO (111,222),ISTRT
C
      111 CONTINUE
C
C--SPECIFY THE BRINE MASS (AMB) FROM THE TC FILL RECORDS AND THE
C BRINE MOLECULAR WEIGHT (WTMOLB). THEN COMPUTE THE MOLES OF
C BRINE IN THE TC (ANB).
C
C NOTE: THE QUANTITY OF BRINE IS THE ACTUAL QUANTITY, WHEREAS
C THE VOLUME OF "LIQUID" USED IN OTHER PARTS OF THE PROGRAM
C ACCOUNT FOR THE WASTE AS WELL, SO THAT THE BETA COEFFICIENT
C AND VOLUME FOR THE "LIQUID" FOUND THERE REFERS TO THE
C COMBINATION OF BRINE AND WASTE

```

```

C
      READ (4,3) AMB,WTMOLB
      3 FORMAT(/2E10.0)
      ANB=AMB/WTMOLB
C
C--SPECIFY THE UNIVERSAL GAS CONSTANT (RU) AND THE STANDARD
C ATMOSPHERIC PRESSURE (PATM) IN CONSISTENT UNITS - EG, WITH
C [T]=K, [P]=PSIA, [VS]=ML, [AMB]=G, & [WTMOLB]=G/GMOLE THEN
C PATM=14.696 PSIA & RU=1205.95 PSIA*ML/GMOLE/K
      READ (4,4) RU,PATM
      4 FORMAT(/2E10.0)
C
C--SPECIFY THE VOLUMETRIC FRACTION (VFRG), MOLECULAR WT (WTMOLG)
C AND THE ASSOCIATED SOLUBILITY PARAMETERS A,B, & C PER THE
C RELATIONS CITED IN CRC HANDBOOK OF CHEMISTRY & PHYSICS FOR THE
C SOLUBLE GAS [VFRG = 0. GIVES THE INSOLUBLE-GAS RESULTS].
C
C--NOTE: THE CURRENT FORMULATION DOES NOT ACCOUNT FOR CHANGES IN
C THE TOTAL MASS (HS + DISSOLVED) OF SOLUBLE GAS SPECIES WITHIN
C THE TEST CONTAINER THAT RESULTS FROM GAS GENERATION
C
      READ (4,1) VFRG,A,B,C
      1 FORMAT(/4E10.0)
C
      WRITE(10,2) AMB,ANB,WTMOLB,RU,PATM,VFRG,A,B,C
      2 FORMAT(/'SOLUBILITY PARAMETERS:'/5X,'AMB=',4PE15.4/5X,
      1 'ANB=',3PE15.4/5X,'WTMOLB=',E12.4/5X,'RU=',4PE15.4/5X,
      2 'PATM=',F8.3/5X,'VFRG=',E12.4/5X,'A,B,C=',3E15.5)
C
      222 CONTINUE
C
C--COMPUTE THE MOLE FRACTION OF THE GAS SPECIES DISSOLVED IN THE
C BRINE AT ONE ATMOSPHERE PARTIAL PRESSURE IN THE HS (X) FOR THE
C THE PRESENT CONDITIONS
      TSTAR=(TB+273.15)/100.
      ALNX=A+B/TSTAR+C*ALOG(TSTAR)
      X=EXP(ALNX)
C
C--USE HENRY'S LAW TO ACCOUNT FOR THE ACTUAL PARTIAL PRESSURE
C (PPRES) OF THE SOLUBLE GAS SPECIES WITHIN THE HS [THE PARTIAL
C PRESSURE OF A SPECIE EQUALS THE VOL FRACTION TIMES THE TOTAL
C PRESSURE OF ALL GASES WITHIN THE HS]
      PPRES=VFRG*PG
C
C DETERMINE THE MOLE FRACTION OF THE DISSOLVED GAS SPECIES IN
C SOLUTION AT THE ACTUAL GAS PRESSURE (SX) AND THE ACTUAL NUMBER

```

```

C   OF MOLES OF DISSOLVED GAS (ANDIS), AND CALCULATE R(UNIV)*ANDIS
      SX=X*PPRES/PATM
      ANDIS=ANB*SX/(1.-SX)
      RUNDIS=RU*ANDIS
C
      WRITE(10,5)PPRES,X,SX,ANDIS,RUNDIS
5  FORMAT(/5X,'SOLUBILITY CALCULATION: '/5X,'PPRES=',E12.4/5X,
1  'X=',E12.4/5X,'SX=',E12.4/5X,'ANDIS=',E12.4/5X,'RUNDIS=',
2  E12.4)
C
      RETURN
      END
C-----
-
C-----
-
C   PROGRAM ONEDIM
      SUBROUTINE ONEDIM(ISTRT,TRTD,TGB,TGBEX,TTILDA)
C
C   AUTHOR: F.S. FELICIONE, ANL-W
C
C   GGE VERSION 007, 06-2001: ACCOUNT FOR 2-D EFFECTS IN THE HEAD
C   BY USING 2X THE CONDUCTANCE IN HEADSPACE AND 5.00X IN HEAD &
C   SURFACE IN S/R XPORT
C
C   THIS PROGRAM USES THE MEASURED GGE CONTAINER AND GLOVEBOX
C   TEMPERATURES TO CALCULATE THE STEADY-STATE TEMPERATURE IN THE
C   HEADSPACE OF THE CONTAINERS VIA A 1-DIMENSIONAL ANALYSIS
C
      COMMON/ALL/TAR(5),THD(5),THS(5),TBW(5)
1  ,AKAR(5),AKHD(5),AKHS(5),AKBW(5),VAR(5),VHS(5),VBW(5)
2  ,CAR(5),CHS(5),CBW(5),RAR(5),RHS(5),RBW(5)
3  ,TINF,T0,T1,T2,T3,H0,HA,HB,HC,AL0,AL1,AL2,AL3,AL4,AL5,AL6
4  ,PR,NAR,NHD,NHS,NBW,ICONVG
C
      COMMON/TEMP/TEXGLB
C
C--ESTABLISH PROGRAM-ENTRY POINT
      GO TO (221,222), ISTRT
C
221 CONTINUE
C
      OPEN (UNIT=4,FILE='C:\RMFORT\DATASET\ONEDIM.TXT',
C   1  STATUS='OLD', BLANK='ZERO')
C   OPEN (UNIT=10,FILE='C:\RMFORT\OUTPUT\ONEDIM.OUT',
C   1  STATUS='UNKNOWN')

```

```

C
C--PRINT HEADER
C      WRITE(10,6)
      6 FORMAT(18X,'GAS-GENERATION EXPERIMENTS' /
      1 19X,'ONE-DIMENSIONAL ANALYSIS'//)
C
C--INPUT GEOMETRY OF THE HEAT-FLOW-PATH STRUCTURE (REF. FSF NOTE,
C "REVERT TO 1-D MODEL", 10-98)
      READ (4,1) AL0,AL1,AL2,AL3,AL4,AL5,AL6
      1 FORMAT(///(5E10.0))
C      WRITE (10,5) AL0,AL1,AL2,AL3,AL4,AL5,AL6
      5 FORMAT(/'REGION LENGTHS'/5X,'L0=',E12.4/5X,'L1=',E12.4/
      1 5X,'L2=',E12.4/5X,'L3=',E12.4/5X,'L4=',E12.4/
      2 5X,'L5=',E12.4/5X,'L6=',E12.4)
C
C--INPUT THERMOPHYSICAL PROPERTIES
C
      CALL PROPTBL
C
C--SPECIFY TEMP CONVERGENCE TOLERANCE AND RESUBSTITUTION CYCLES
C LIMIT {DTERR & LIMIT}
      READ(4,16)LIMIT,DTERR
      16 FORMAT(/I5,5X,E10.0)
C      WRITE (10,15)DTERR
      15 FORMAT(/'CONVERGENCE TOLERANCE=',F8.4)
C
      RETURN
C
222 CONTINUE
C
C--INPUT GGE TEMPERATURE MEASUREMENTS, AND THE EXCESS TEMPERATURE
C OVER TGB {TGBEX}, TO ACCOUNT FOR THE APPROPRIATE ACTUAL TC
C ENVIRONMENT TEMPERATURE VARIATION FROM THE MEASURED TGB VALUE
C
      READ (4,2) TRTD,TGB,TGBEX
      2 FORMAT(/3E10.0)
      WRITE (10,11) TRTD,TGB,TGBEX
      11 FORMAT(/5X,'TEMP DATA & ASSUMED TEMP EXCESS OVER GB'
      1 /5X,'TRTD=',F6.2,5X,'TGB=',F6.2,5X,'TGBEX=',F6.2)
C
      TINF=TGB+TGBEX+TEXGLB
C
C--BYPASS THE TG DETERMINATION IF THE DIFFERENCE BETWEEN TRTD AND
C TINF IS LESS THAN A QUANTITY DIF OR IF TINF EXCEEDS TRTD
      DIF=0.001
      IF(TRTD-(TINF+DIF)) 17,17,18

```



```

17 TTILDA=TRTD
   RETURN
C
18 CONTINUE
C
C--GUESS AN INITIAL TEMPERATURE DISTRIBUTION SUCH THAT
C (T2+T3)/2=TRTD
C   READ (4,3) T0,T1,T2,T3
C   3 FORMAT(/4E10.0)
C
C   TSPRED=TRTD-TINF
C   T0=TINF+0.3*TSPRED
C   T1=T0+0.3*TSPRED
C   T2=T1+0.2*TSPRED
C   T3=TRTD+0.2*TSPRED
C
C   WRITE (10,12) TINF,T0,T1,T2,T3
12 FORMAT(/5X,'INITIAL ASSUMED TEMPERATURE DISTRIBUTION'/
1   5X,'TINF=',F6.2/5X,'T0=',F8.2/5X,'T1=',F8.2/5X,'T2=',
2   F8.2/5X,'T3=',F8.2)
C
C--CALCULATE THE THERMAL CONDUCTANCES APPLICABLE TO THE ASSUMED
C TEMPERATURE DISTRIBUTION
C
C--LOOP THE TEMPERATURE-DISTRIBUTION CALCULATION, USING
C SUCCESSIVE SUBSTITUTION OF THE COMPUTED TEMPERATURES UNTIL ALL
C TEMPERATURES VARY LESS THAN A USER-SPECIFIED TOLERANCE, DTERR.
C UP TO 'LIMIT' SUBSTITUTIONS ARE ATTEMPTED, WHERE LIMIT IS USER
C SPECIFIED
C
C--THE CONVERGENCE INDICATOR, ICONVG, INHIBITS WRITING OF
C PARAMETERS UNTIL CONVERGENCE IS REACHED; THEN ONE MORE CYCLE
C IS MADE, AND PARAMETERS ARE WRITTEN
C   ICONVG=0
C   DO 999 ILOOP=1,LIMIT
C
C   T0P=T0
C   T1P=T1
C   T2P=T2
C   T3P=T3
C
C   CALL XPORT
C
C   IF(ICONVG .EQ. 1)WRITE(10,9)HC,HB,HA,H0
9   FORMAT(/5X,'REGION CONDUCTANCES'/
1   5X,'HC=',F8.3/5X,'HB=',F8.3/5X,'HA=',F8.3/5X,'H0=',F8.3)

```

```

C
C--COMPUTE TEMPERATURE DISTRIBUTION
  ONEDH=1./HC+1./HB+1./HA+1./H0
  BRACK=1./HC/ONEDH
  T2=(2.*TRTD*(BRACK-1.)-BRACK*TINF)/(BRACK-2.)
  T3=2.*TRTD-T2
  Q=(T3-TINF)/ONEDH
  T0=TINF+Q/H0
  T1=T2-Q/HB
  TTILDA=T1+(T2-T1)/3.

C
  IF(ICONVG .EQ. 1)WRITE(10,8)ILOOP,TINF,TRTD,T0,T1,T2,T3,
1  TTILDA
8  FORMAT(/5X,'ONEDIM TEMP DIST DETERMINATION, CYCLE NO.',I3/
1  5X,'TINF',F9.3/5X,'TRTD',F9.3/5X,'T0',F11.3/
2  5X,'T1',F11.3/5X,'T2',F11.3/5X,'T3',F11.3/5X,'TTILDA',
3  F7.3)

C
C--TEST CONVERGENCE
  IF(ABS(T0-T0P) .GT. DTERR)GO TO 999
  IF(ABS(T1-T1P) .GT. DTERR)GO TO 999
  IF(ABS(T2-T2P) .GT. DTERR)GO TO 999
  IF(ABS(T3-T3P) .GT. DTERR)GO TO 999

C
  IF(ICONVG .EQ. 1)RETURN
  ICONVG=1
  WRITE (10,14)
14  FORMAT(/5X,'CONVERGENCE OF ALL TEMPERATURES ACHIEVED')

C
999  CONTINUE
  STOP'CONVERGENCE NOT ACHIEVED IN ONEDIM'
  END

C-----
-
C-----
-

  SUBROUTINE PROPTBL

C
  COMMON/ALL/TAR(5),THD(5),THS(5),TBW(5)
1  ,AKAR(5),AKHD(5),AKHS(5),AKBW(5),VAR(5),VHS(5),VBW(5)
2  ,CAR(5),CHS(5),CBW(5),RAR(5),RHS(5),RBW(5)
3  ,TINF,T0,T1,T2,T3,H0,HA,HB,HC,AL0,AL1,AL2,AL3,AL4,AL5,AL6
4  ,PR,NAR,NHD,NHS,NBW,ICONVG

C
C--READ THERMOPHYSICAL PROPERTIES
C

```

C	NXX	NO. OF PROPERTY-TABLE POINTS (XXX=AR,N2,ETC.)
C	AKXX	THERMAL CONDUCTIVITY
C	VXX	KINEMATIC VISCOSITY
C	CXX	HEAT CAPACITY (CONST. PRESS)
C	RXX	MASS DENSITY
C	AR	ARGON GAS
C	HD	TEST CONTAINER HEAD
C	HS	HEADSPACE GAS
C	BW	BRINE/WASTE

C

```

      READ (4,1) NAR,(TAR(I),AKAR(I),VAR(I),CAR(I),RAR(I),
1  I=1,NAR)
1  FORMAT (/I5/(5E10.0))
C      WRITE (10,3) (TAR(I),AKAR(I),VAR(I),CAR(I),RAR(I),I=1,NAR)
3  FORMAT(/'ARGON PROPERTY TABLE {T,K,V,C,R}' /
1  (5X,F6.2,4(3X,E10.3)))

```

C

```

      READ (4,2) NHD,(THD(I),AKHD(I),I=1,NHD)
2  FORMAT (/I5/(2E10.0))
C      WRITE (10,4) (THD(I),AKHD(I),I=1,NHD)
4  FORMAT(/'TC HEAD CONDUCTIVITY TABLE' /
1  (5X,F6.2,3X,E10.3))

```

C

```

      READ (4,1) NHS,(THS(I),AKHS(I),VHS(I),CHS(I),RHS(I),
1  I=1,NHS)
C      WRITE (10,5) (THS(I),AKHS(I),VHS(I),CHS(I),RHS(I),I=1,NHS)
5  FORMAT(/'HEADSPACE-GAS PROPERTY TABLE {T,K,V,C,R}' /
1  (5X,F6.2,4(3X,E10.3)))

```

C

```

      READ (4,1) NBW,(TBW(I),AKBW(I),VBW(I),CBW(I),
1  RBW(I),I=1,NBW)
C      WRITE (10,6) (TBW(I),AKBW(I),VBW(I),CBW(I),RBW(I),I=1,NBW)
6  FORMAT(/'BRINE/WASTE PROPERTY TABLE {T,K,V,C,R}' /
1  (5X,F6.2,4(3X,E10.3)))

```

C

```

      RETURN
      END

```

C-----

-

C-----

-

```

      SUBROUTINE XPORT

```

C

```

      COMMON/ALL/TAR(5),THD(5),THS(5),TBW(5)
1  ,AKAR(5),AKHD(5),AKHS(5),AKBW(5),VAR(5),VHS(5),VBW(5)
2  ,CAR(5),CHS(5),CBW(5),RAR(5),RHS(5),RBW(5)

```

```

      3 ,TINF,T0,T1,T2,T3,H0,HA,HB,HC,AL0,AL1,AL2,AL3,AL4,AL5,AL6
      4 ,PR,NAR,NHD,NHS,NBW,ICONVG
C
C      TAVE      AVERAGE TEMPERATURE
C      DIFXX     THERMAL DIFFUSIVITY
C      BETAXX    THERMAL EXPANSION COEFFICIENT
C      RAXX      RAYLEIGH NUMBER
C      PRXX      PRANDTL NUMBER
C      RACXX     CRITICAL RAYLEIGH NO.
C      RACIXX    SPECIFIC CRITICAL RAYLEIGH NO.
C
C--DETERMINE CONDUCTANCE VALUES IN BRINE/WASTE (BW),
C HEADSPACE GAS (HS), TC HEAD (HD), AND TC SURFACE (AR)
C
C--BRINE/WASTE
C
      TAVE=(T2+T3)/2.
      DTBW=T3-T2
      CALL TBLKUP(TAVE,NBW,TBW,AKBW,VBW,CBW,RBW,AKVBW,
1  VVBW,CVBW,RVBW)
C
      DIFBW=AKVBW/RVBW/CVBW
C
C--LINEARIZE BRINE/WASTE BETA DATA
      TBETAL=20.
      BETAL=0.355E-3
      TBETAH=40.
      BETAH=0.394E-3
      BETABW=BETAL+(TAVE-TBETAL)/(TBETAH-TBETAL)*(BETAH-BETAL)
C
C      IF(ICONVG .EQ. 1)WRITE(10,23)TAVE,AKVBW,VVBW,CVBW,RVBW,
C      1  DIFBW,BETABW
23  FORMAT(/5X,'BRINE/WASTE PROP {K,V,C,R,D,BETA} TAVE=',F6.2
1  /(2X,4(3X,E10.4)))
C
      CALL RAYLEE(BETABW,AL6,VVBW,DIFBW,DTBW,RABW,PRBW)
      IF(ICONVG .EQ. 1)WRITE(10,21)RABW,PRBW
21  FORMAT(/5X,'RA=',E10.3,5X,'PR=',E10.3)
C
      RACIBW=19494.
      RACBW=RACIBW
C
      CALL NUSSLT(RABW,PRBW,RACBW,AL6,AKVBW,HC)
C
C--HEADSPACE GAS
C

```

```

      TAVE=(T1+T2)/2.
      DTHS=T2-T1
      CALL TBLKUP(TAVE,NHS,THS,AKHS,VHS,CHS,RHS,AKVHS,
1    VVHS, CVHS, RVHS)
C
      DIFHS=AKVHS/RVHS/CVHS
      BETAHS=1./(TAVE+273.16)
C
C    IF(ICONVG .EQ. 1)WRITE(10,24)TAVE,AKVHS,VVHS, CVHS, RVHS,
C    1    DIFHS,BETAHS
24  FORMAT(/5X,'HS-GAS PROPERTIES {K,V,C,R,D,BETA} AT TAVE=',
1    F6.2/(2X,4(3X,E10.4)))
C
      CALL RAYLEE(BETAHS,AL2,VVHS,DIFHS,DTHS,RAHS,PRHS)
C    IF(ICONVG .EQ. 1)WRITE(10,20)RAHS,PRHS
20  FORMAT(/5X,'RA=',E10.3,5X,'PR=',E10.3)
C
      RACIHS=1860.4
      RACHS=RACIHS
C
      CALL NUSSLT(RAHS,PRHS,RACHS,AL2,AKVHS,HB)
C
C--MAKE ADJUSTMENT FOR 2-D EFFECTS
      HB=2.*HB
C
C--TC HEAD
C
      TAVE=(T0+T1)/2.
      IF(NHD .EQ. 1)GO TO 8
      N=NHD-1
      DO 5 I=1,N
      IF(TAVE .GE. THD(I) .AND. TBAR .LE. THD(I+1))GO TO 7
5    CONTINUE
      WRITE(10,6)
6    FORMAT(//'TEMPERATURE OUTSIDE OF HD-PROPERTY-TABLE RANGE')
      STOP'TEMP OUTSIDE OF HD-PROP TABLE RANGE, S/R XPORT'
C
7    CONTINUE
      TFAC=(TAVE-THD(I))/(THD(I+1)-THD(I))
      AKVHD=AKHD(I)+TFAC*(AKHD(I+1)-AKHD(I))
      GO TO 9
C
8    CONTINUE
      AKVHD=AKHD(1)
C
9    CONTINUE

```

```

C      IF(ICONVG .EQ. 1)WRITE(10,25)TAVE,AKVHD
25  FORMAT(/5X,'TC HEAD THERMAL CONDUCTIVITY {K} AT TAVE=',
1    F6.2/(2X,4(3X,E10.4)))
      HA=AKVHD/AL1
C
C--MAKE ADJUSTMENT FOR 2-D EFFECTS
      HA=5.00*HA
C
C--ARGON GAS
      TAVE=(TINF+T0)/2.
      DTAR=T0-TINF
      CALL TBLKUP(TAVE,NAR,TAR,AKAR,VAR,CAR,RAR,AKVAR,
1    VVAR,CVAR,RVAR)
C
      BETAAR=1./(TAVE+273.16)
      DIFAR=AKVAR/CVAR/RVAR
C
C      IF(ICONVG .EQ. 1)WRITE(10,26)TAVE,AKVAR,VVAR,CVAR,RVAR,
C      1  DIFAR,BETAAR
26  FORMAT(/5X,'ARGON GAS PROP {K,V,C,R,D,BETA} TAVE=',F6.2
1    /(2X,4(3X,E10.4)))
C
      CALL RAYLEE(BETAAR,AL0,VVAR,DIFAR,DTAR,RAAR,PRAR)
C      IF(ICONVG .EQ. 1)WRITE(10,22)RAAR,PRAR
22  FORMAT(/5X,'RA=',E10.3,5X,'PR=',E10.3)
C
      CLBAR=0.515
      ANUT=0.835*CLBAR*RAAR**0.25
      ANU=1.4/ALOG(1.+1.4/ANUT)
      H0=ANU*AKVAR/AL0
C
C--MAKE ADJUSTMENT FOR 2-D EFFECTS
      H0=5.00*H0
C
      RETURN
      END
C-----
-
C-----
-
      SUBROUTINE TBLKUP(TBAR,NPTS,T,AK,V,C,R,AKV,
1    VV,CV,RV)
C
      COMMON/ALL/TAR(5),THD(5),THS(5),TBW(5)
1    ,AKAR(5),AKHD(5),AKHS(5),AKBW(5),VAR(5),VHS(5),VBW(5)
2    ,CAR(5),CHS(5),CBW(5),RAR(5),RHS(5),RBW(5)

```

```

      3 ,TINF,T0,T1,T2,T3,H0,HA,HB,HC,AL0,AL1,AL2,AL3,AL4,AL5,AL6
      4 ,PR,NAR,NHD,NHS,NBW,ICONVG
C
      DIMENSION T(1),AK(1),V(1),C(1),R(1)
C
      IF(NPTS .EQ. 1)GO TO 5
C
      N=NPTS-1
      DO 2 I=1,N
      IF(TBAR .GE. T(I) .AND. TBAR .LE. T(I+1))GO TO 3
2 CONTINUE
      WRITE(10,4)
      4 FORMAT(// 'TEMPERATURE OUTSIDE OF PROPERTY TABLE RANGE')
      WRITE(9,6) TBAR
      6 FORMAT('TBAR= ',E12.4)
      STOP'TEMP OUT OF PROP TABLE RANGE, S/R TBLKUP'
C
      3 CONTINUE
      TFAC=(TBAR-T(I))/(T(I+1)-T(I))
      AKV= AK(I)+TFAC*(AK(I+1)-AK(I))
      VV=V(I)+TFAC*(V(I+1)-V(I))
      CV=C(I)+TFAC*(C(I+1)-C(I))
      RV=R(I)+TFAC*(R(I+1)-R(I))
      RETURN
C
      5 CONTINUE
      AKV=AK(1)
      VV=V(1)
      CV=C(1)
      RV=R(1)
C
      RETURN
      END
C-----
-
C-----
-
      SUBROUTINE RAYLEE(BETA,AL,VIS,DIFF,DT,RA,PR)
C
      G=9.81
      GR=G*BETA*DT*AL**3/VIS**2
      PR=VIS/DIFF
      RA=GR*PR
C
      RETURN
      END

```

```

C-----
-
C-----
-
      SUBROUTINE NUSSLT(RA,PR,RAC,AL,AK,H)
C
C--REFERENCE: ROHSENOW, HARTNETT, & GANIC, "HANDBOOK OF HEAT-
C  TRANSFER FUNDAMENTALS", 2ND ED. (HHTF), P. 6-45.
C
C--COMPUTE THE K1 AND K2 FACTORS PER HHTF
      AK1=1.44/(1.+0.018/PR+0.00136/PR**2)
      AK2=75.*EXP(1.5/(PR**0.5))
C
C--COMPUTE THE NUSSELT VALUE TERMS
      TERM1=1.-RAC/RA
      TERM1=(ABS(TERM1)+TERM1)/2.
C
      TERM2=(RA/5380.）**0.33333-1.
      TERM2=(ABS(TERM2)+TERM2)/2.
C
      TERM3=(RA**0.33333)/AK2
C
      TERM4=(RA/RAC)**0.33333-1.
      TERM4=(ABS(TERM4)+TERM4)/2.
C
C--COMPUTE THE NUSSELT NUMBER (ANU)
      ANU=1.+TERM1*(AK1+2.*TERM3**(1.-ALOG(TERM3)))+
1  TERM2*(1.-EXP(-0.95*TERM4))
      H=ANU*AK/AL
C
      RETURN
      END
C-----
-
C-----
-
      SUBROUTINE BB(ISTRT,T,P,Z)
C
C--THIS PROGRAM SOLVES THE EQUATION OF STATE FOR A NON-IDEAL
C  GAS USING THE BEATTIE-BRIDGEMAN EQUATION (REF: VAN WYLEN,
C  THERMODYNAMICS, TABLE 14.1) FOR A SPECIFIED TEMPERATURE AND
C  GAS PRESSURE. A COMPRESSIBILITY FACTOR, Z, IS THEN COMPUTED
C  TO ALLOW THE STATE EQUATION TO BE REPRESENTED AS PV=ZMRT.
C
C--SINCE THE BEATTIE-BRIDGEMAN EQN IS TRANSCENDENTAL, A TRIAL
C  SOLUTION IS USED: SPECIFIC VOLUME IS GUESSED AND THE RESULTING

```



```

C  PRESSURE IS COMPUTED.  THIS IS COMPARED TO THE ACTUAL PRESSURE
C  TO DETERMINE CONVERGENCE.  ONCE CONVERGENCE HAS BEEN ACHIEVED,
C  THE COMPRESSIBILITY FACTOR IS CALCULATED AS  $Z=Pv/RT$ .
C
C  INPUT UNITS ARE TEMP: C
C                      PRESS: PSIA
C  CONSTANTS AND OUTPUT ARE IN ATM,1/GMOLE,AND K
C
C--THE CONSTANTS BELOW PERTAIN ONLY TO NITROGEN; OTHER CONSTANTS
C  ARE NEEDED FOR OTHER GASES (SEE REF).  AN 'S' AS SECOND
C  CHARACTER IDENTIFIES LOWERCASE LETTER, AS USED IN THE
C  REFERENCE.
C
C      GO TO (221,222),ISTRT
C
221 CONTINUE
    A0=1.3445
    AS=0.02617
    B0=0.05046
    BS=-6.910E-3
    CS=42000.
    R=0.08206
C
    WRITE(10,15) A0,B0,AS,BS,CS,R
15  FORMAT(/'BEATTIE-BRIDGEMAN EQN CONSTANTS:'
1    /5X,'A0',E14.5/5X,'B0',E14.5/5X,'AS',E14.5/5X,'BS',E14.5
2    /5X,'CS',E14.5/5X,'R',E15.5)

C--SPECIFY THE SPECIFIC VOLUME RANGE TO BE USED AND THE NUMBER OF
C  ROUGH INCREMENTS WITHIN THE RANGE.  FIRST, A ROUGH SCREENING
C  IS PERFORMED TO LOCATE THE APPLICABLE INTERVAL; THEN A FINE
C  SCREENING IS PERFORMED WITHIN THIS INTERVAL USING THE SAME
C  NUMBER OF INCREMENTS.  FINALLY, A LINEAR FIT TO THE CORRECT
C  FINE INTERVAL IS MADE TO DETERMINE THE SOLUTION.
C
C      V          SPECIFIC VOLUME
C      VTBLO      LOW VALUE FROM V-INPUT TABLE
C      VTBHI      HIGH VALUE FROM V-INPUT TABLE
C      VLO        LOW VALUE FOR V RANGE
C      VHI        HIGH VALUE FOR V RANGE
C      NUM        NUMBER OF INCREMENTS WITHIN THE RANGE
C
    READ(4,1) NUM,VTBLO,VTBHI
1  FORMAT(/I5,5X,2E10.0)
    WRITE(10,12) NUM,VTBLO,VTBHI
12  FORMAT(/'V-TABLE:',I4,' INCREMENTS.  LOW V = ',E10.3,3X,

```

```

1 'HI V = ',E10.3)
C
    RETURN
C
C--THE CHARACTERISTIC OF THE B-B EQUATION IS THAT A SPECIFIC
C VOLUME GUESS THAT IS TOO LOW WILL YIELD A CALULATED
C PRESSURE THAT EXCEEDS THE ACTUAL PRESSURE; CONVERSELY, IF THE
C SPECIFIC VOLUME USED IS TOO HIGH, THE CALCULATED PRESSURE IS
C LESS THAN THE ACTUAL PRESSURE. BUT THIS TREND SHOULD BE HAND
C VERIFIED FOR OTHER GASES BEFORE USING THIS ROUTINE.
C
C--CALCULATE THE IMPLIED PRESSURE. THE FIRST TIME THROUGH IS A
C ROUGHING CALCULATION TO LOCATE THE PROPER INTERVAL; THE SECOND
C TIME THROUGH IS A FINE CALCULATION.
C
222 CONTINUE
    WRITE(10,16)T,P
    16 FORMAT(/5X,'COMPRESSIBILITY AT',2X,'T=',F6.2,' & P=',F9.2)
C
    WRITE (10,3)
    3 FORMAT(/10X,'V',15X,'PCALC',10X,'RATIO')
C
C--CONVERT [T]=C TO [TK]=K, AND [P]=PSIA TO [PA]=ATM
    TK=273.15+T
    PA=P/14.696
C
    DV=(VTBHI-VTBLO)/NUM
    V=VTBLO
    NUMP1=NUM+1
C
    DO 2 I=1,NUMP1
    V1=V
    IF(I .GT. 1)V=V+DV
    A=A0*(1.-AS/V)
    B=B0*(1.-BS/V)
    E=CS/V/TK**3
    PCALC=(R*TK*(1.-E)*(V+B)-A)/V**2
    RATIO=PCALC/PA
C
    WRITE(10,5) V,PCALC,RATIO
    5 FORMAT(4X,3E15.7)
C
    WRITE(10,13) A,B,E
    13 FORMAT(10X,'A,B,E:',5X,E13.7,2E15.7)
C
C--DETERMINE IF THE SOLUTION (RATIO = 1) LIES BETWEEN THIS V
C VALUE AND THE PREVIOUS VALUE: RATIO > 1 MEANS THE CORRECT
C INTERVAL NOT YET REACHED; THE FIRST RATIO < 1 MEANS THAT THE

```

```

C  CORRECT INTERVAL HAS BEEN FOUND.
    IF(RATIO .GT. 1.)GO TO 2
    IF(RATIO .EQ. 1.)GO TO 8
    VLO=V1
    VHI=V
    GO TO 4
2  CONTINUE
    STOP 'INITIAL V-TABLE RANGE INSUFFICIENT'
C
    4  CONTINUE
C
C--NOW PERFORM FINE SCREENING OVER THE INTERVAL FOUND ABOVE
C    WRITE(10,17)
17  FORMAT(/5X,'FINE SCREENING')
    DV=(VHI-VLO)/NUM
    V=VLO
C
    DO 6 I=1,NUMP1
    V1=V
    IF(I .GT. 1)RAT1=RATIO
    IF(I .GT. 1)V=V+DV
    A=A0*(1.-AS/V)
    B=B0*(1.-BS/V)
    E=CS/V/TK**3
    PCALC=(R*TK*(1.-E)*(V+B)-A)/V**2
    RATIO=PCALC/PA
C    WRITE(10,11) V,PCALC,RATIO
11  FORMAT(4X,3E15.7)
C
C--DETERMINE IF THE SOLUTION LIES BETWEEN THIS V VALUE AND THE
C PREVIOUS VALUE
    IF(RATIO .GT. 1.)GO TO 6
    IF(RATIO .EQ. 1.)GO TO 8
    V2=V
    RAT2=RATIO
    GO TO 7
6  CONTINUE
    STOP 'FINE INTERVAL NOT YIELDING SOLUTION'
C
    7  CONTINUE
C--NOW LINEARLY INTERPOLATE OVER THIS INTERVAL TO DETERMINE
C SOLUTION FOR V
    V=V1+(V2-V1)*(1.-RAT1)/(RAT2-RAT1)
C
    8  CONTINUE
C--SOLUTION OF STATE EQN FOUND, CALCULATE Z AND WRITE

```

```

A=A0*(1.-AS/V)
B=B0*(1.-BS/V)
E=CS/V/TK**3
PCALC=(R*TK*(1.-E)*(V+B)-A)/V**2
RATIO=PCALC/PA
Z=PCALC*V/R/TK
WRITE(10,9)V,RATIO,Z
9  FORMAT(/5X,'V',E19.7/5X,'RATIO',E15.7/5X,'Z',E19.7)
C
RETURN
END

```