S	ENGINEERING CHANGE NOTICE	Page 1 of <u>2</u>	1. ECN 655274 Proj. ECN
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2. ECN Category (mark one) Supplemental ☐ Direct Revision ☒ Change ECN ☐ Temporary ☐ Standby ☐ Supersedure ☐ Cancel/Void ☐	3. Originator's Name, Organization, MSIN, and Telephone No. M.J. Packer/Process Engineering/R3-86/376-6625	4. USQ Required? ☒ Yes ☐ No	5. Date 1/4/00
	6. Project Title/No./Work Order No. Spent Nuclear Fuel Project	7. Bldg./Sys./Fac. No. N/A	8. Approval Designator Sn/Q
	9. Document Numbers Changed by this ECN (includes sheet no. and rev.) HNF-4301, Rev. 1	10. Related ECN No(s). N/A	11. Related PO No. N/A
12a. Modification Work ☐ Yes (fill out Blk. 12b) ☒ No (NA Blks. 12b, 12c, 12d)	12b. Work Package No. N/A	12c. Modification Work Completed N/A Design Authority/Cog. Engineer Signature & Date	12d. Restored to Original Condition (Temp. or Standby ECNs only) N/A Design Authority/Cog. Engineer Signature & Date

13a. Description of Change
 Sections 20, 21, 22, and Appendix S are added to HNF-4301, Rev. 1.

13b. Design Baseline Document? ☐ Yes ☒ No

Record of Revision page - title change from 'MCO Gas composition for Low Reactive Surface Areas' to 'Gas Composition Transients in the Vacuum Drying Facility.'

Document re-formatted per Section in Table of Contents. Also includes list of Figures and Tables. Page numbers changed from overall numerical increase to numerical increase per Section.

The added sections are continued confirmation bases for selected problems involving the prediction of transient gas compositions during Cold Vacuum Drying Operations.

EDT 626803, DET 626115, and EDT 627108 include design equations and plotting routines with associated inputs which support HNF-4301, Rev. 2. EDT 626803 includes Sections 1-9, EDT 626115 includes Sections 10-19, and EDT 627108 includes Section 20-22 in HNF-4301, Rev. 2.

USQ-Like: CVD-00-001780
 usq # K-00-0098

14a. Justification (mark one) Criteria Change ☐ Design Improvement ☒ Environmental ☐ Facility Deactivation ☐ As-Found ☐ Facilitate Const. ☐ Const. Error/Omission ☐ Design Error/Omission ☐	14b. Justification Details Continued selected problems with associated confirmation bases added to HNF-4301, Rev. 1. Review checklist for HNF-4301, Rev. 2 is in EDT 626811, EDT 626302, and EDT 627593. 628125 <i>MJP</i> 3/14/00
--	---

15. Distribution (include name, MSIN, and no. of copies)
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Page 2 of 2

1. ECN (use no. from pg. 1)

655274

16. Design Verification Required

☐ Yes

☒ No

17. Cost Impact *N/A* ENGINEERING

Additional ☐ \$ _____

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CONSTRUCTION

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18. Schedule Impact (days)

N/A

Improvement ☐ _____

Delay ☐ _____

19. Change Impact Review: Indicate the related documents (other than the engineering documents identified on Side 1) that will be affected by the change described in Block 13. Enter the affected document number in Block 20.

SDD/DD	☐	Seismic/Stress Analysis	☐	Tank Calibration Manual	☐
Functional Design Criteria	☐	Stress/Design Report	☐	Health Physics Procedure	☐
Operating Specification	☐	Interface Control Drawing	☐	Spares Multiple Unit Listing	☐
Criticality Specification	☐	Calibration Procedure	☐	Test Procedures/Specification	☐
Conceptual Design Report	☐	Installation Procedure	☐	Component Index	☐
Equipment Spec.	☐	Maintenance Procedure	☐	ASME Coded Item	☐
Const. Spec.	☐	Engineering Procedure	☐	Human Factor Consideration	☐
Procurement Spec.	☐	Operating Instruction	☐	Computer Software	☐
Vendor Information	☐	Operating Procedure	☐	Electric Circuit Schedule	☐
OM Manual	☐	Operational Safety Requirement	☒	ICRS Procedure	☐
FSAR/SAR	☒	IEFD Drawing	☐	Process Control Manual/Plan	☐
Safety Equipment List	☐	Cell Arrangement Drawing	☐	Process Flow Chart	☐
Radiation Work Permit	☐	Essential Material Specification	☐	Purchase Requisition	☐
Environmental Impact Statement	☐	Fac. Proc. Samp. Schedule	☐	Tickler File	☐
Environmental Report	☐	Inspection Plan	☐		☐
Environmental Permit	☐	Inventory Adjustment Request	☐		☐

20. Other Affected Documents: (NOTE: Documents listed below will not be revised by this ECN.) Signatures below indicate that the signing organization has been notified of other affected documents listed below.

Document Number/Revision

Document Number/Revision

Document Number/Revision

N/A

N/A

N/A

21. Approvals

Signature

Date

Signature

Date

Design Authority

Cog. Eng. *M. J. Packer*

Cog. Mgr. *J. R. Frederickson*

QA *D. W. Smith*

Safety *R. L. Garrett*

Environ.

Other

Design Agent

PE

QA

Safety

Design

Environ.

Other

DEPARTMENT OF ENERGY

Signature or a Control Number that tracks the Approval Signature

ADDITIONAL

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To Distrubution	From SNF Process Engineering	Page 1 of 1
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HNF-4301
Revision 2
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Gas Composition Transients in the Cold Vacuum Drying Facility

M. J. Packer
Fluor Hanford

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Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

Project Hanford Management Contractor for the
U.S. Department of Energy under Contract DE-AC06-96RL13200

Fluor Hanford
P.O. Box 1000
Richland, Washington

Release Approval
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Gas Composition Transients in the Cold Vacuum Drying Facility

**Prepared for the U.S. Department of Energy
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**Project Hanford Management Contractor for the
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Fluor Hanford
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GAS COMPOSITION TRANSIENTS IN THE COLD VACUUM DRYING FACILITY

Executive Summary

The purpose of this document is to evaluate selected problems involving the prediction of transient gas compositions during Cold Vacuum Drying operations. The problems were evaluated to answer specific design questions. The document is formatted as a topical report with each section representing a specific problem solution. The problem solutions are reported in the calculation format specified in HNF-1613, Rev. 0, EP 7.6.

The problems solutions presented are listed per Section as follows:

1. Evaluation of Helium Purge/Vent to Reduce Hydrogen Gas Concentrations in the MCO and Cask Void Spaces Upon Receipt from K Basin
2. Evaluation MCO Void Gas Composition Prior to Draining
3. Evaluation of Helium Purge Pre-Purge to Reduce Oxygen Concentrations in the PWC Receiving Tanks
4. Evaluation of PWC Receiving Tanks Void Gas Composition During Pre-Purge Delay
5. Evaluation of PWC Receiving Tanks Void Gas Composition Following MCO Bulk Water Drain
6. Evaluation of Helium Purge to Reduce Hydrogen Gas Concentrations in the PWC Receiving Tanks Void Space Following MCO Bulk Water Drain
7. Evaluation of Helium Purge to Reduce Hydrogen Gas Concentrations in the MCO Void Space Prior to Entering Vacuum Mode
8. Evaluation of Helium Purge to Reduce Hydrogen Gas Concentrations in the MCO Void Space During Vacuum Mode
9. Evaluation to Detect Leaks in MCO or Poor Vacuum Pump Performance During Vacuum Dry Mode Using Minimum Helium Purge Rate
10. Evaluation of Transient Hydrogen and Air Leak Oxygen Concentrations in the MCO Void Space During Bulk Water Drain to Validate SCIC Systems Response Time
11. Evaluation of Transient MCO Void Space Hydrogen and Air Leak Oxygen Concentrations After Bulk Water Drain to Validate SCIC Systems Response Time
12. Evaluation of Minimum Helium Purge to Reduce Hydrogen and Oxygen Concentrations in the MCO Void Space After a Vacuum Line Break

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20. "Non-ideal" Evaluation of Minimum Helium Purge to Reduce Hydrogen and Oxygen Concentration in the MCO void Space After a Vacuum Line Break
21. Calculation of Minimum MCO Helium Purge
22. Evaluation of Adequate Safety Class Helium Gas Bottle Pressure

Additional problems may be evaluated and added to future revisions of this report.

1.0 Evaluation of Helium Purge/Vent to Reduce Hydrogen Gas Concentrations in the MCO and Cask Void Space Upon Receipt from K Basin

1.1 Purpose and Objectives

The purpose of this calculation is to ensure the helium purge and vent design basis is adequate for reducing hydrogen gas in the void spaces of the Cask and MCO after receipt from the K Basin. A number of purge/vent cycles are to be determined, using conservative pressure changes, to reduce the hydrogen gas concentration below 1% (0.01 mole H_2 /mole total gas). The hydrogen production rate is based on the High Nominal rate. Comparison figures using a "best estimate" High Nominal rate are included.

1.2 Summary of Final Results and Conclusions

Overall mass (gram mole or mole) and hydrogen balances were performed around the gas void space of the Cask and MCO (mass balances and mathematical derivations attached - see Appendix A). Twenty cycles each (purge, delay, and vent) are performed. The solution variables, y_1 and y_2 , are used to designate the mole fraction of hydrogen in the Cask and MCO for each cycle, respectively. Six design equations were developed to model gas compositions during the purge/delay/vent operation; in other words, one equation is provided for each operation (purge, delay, and vent cycle) and void space (MCO and Cask). Initial hydrogen mole fractions in both the MCO and Cask void spaces are conservatively assumed to be 0.998 mole H_2 /mole gas. The water in the MCO is assumed to be hydrogen saturated.

The 1% hydrogen gas concentration limit could almost be reached in the Cask void space after 14-15 cycles with the 2 minute time delay after the purge cycle; however, this endpoint could not be reached in the MCO void space. Even with the ideal condition, where no time delay is involved, the hydrogen concentration in the MCO still lies above the 1% limit.

Transient hydrogen gas concentrations using the "Best Estimate" High Nominal hydrogen generation rate show the 1% H_2 limit in the MCO and Cask void space can be reached after 10 purge/delay/vent cycles using the assumed input parameters.

1.3 Assumptions

The MCO/Cask void space, prior to purge cycle, is assumed to have an initial pressure of 0.5 psig. The hydrogen generation rate used is the high nominal value of 1.5×10^{-4} g/sec (Pajunen 1998) for the MCO/Cask receipt. Also included, for comparison, a "best estimate" High Nominal hydrogen generation rate of 5.7×10^{-6} g/sec is used (Pajunen 1998). A helium flow rate used is 1.9 SFCM (Irwin et al 1999). Helium gas (assumed 100% He) is used to purge the Cask and MCO to 35.2 psia (20.5 psig) then vented to 15.2 psia (0.5 psig). The pressure in the MCO and Cask void space is assumed to quickly reach equilibrium with each other as gas is added or removed ($P_{MCO} = P_{Cask}$). The void space gas is assumed to be well-mixed within the separated MCO and Cask regions. It is assumed the temperature-dependent water/uranium reaction creating H_2 is constant at any MCO temperature. It is assumed after each purge cycle there is a two-minute delay prior to the vent cycle to account for operator delay and valve; however, for

comparison, plots are shown where no time delay is included. Perfect mixing of the gases between the MCO and Cask void space is assumed during the delay cycle.

1.4 Software Applications

MATLAB[™] was used to plot analytic solutions (see files in EDT 626803) and to solve and plot the Runge-Kutta (RK) numerical method results. Analytical solutions could be derived for 5 of the 6 ordinary differential equations; however, assuming ideal purge/vent operation with no time delay, only the purge and vent cycle solutions are used for solution comparisons with 3 out of 4 solutions being analytical.

Two sets of solutions were derived and compared. The first set consists of two solutions derived analytically for the purge cycle with one analytical and one numerical solution for the vent cycle. The second set consists of all four numerical solutions (hydrogen fractions during purge and vent in the MCO and Cask) derived by the RK method. These two sets are compared in Figure 1-5 at the 20th cycle for determining approximation error. Figure 1-5 indicates no significant difference exists between the numerical and analytical solutions (note the x's, which denote the RK or numerical solution, is plotted almost directly on top of the continuous line or analytical solution).

The analytical solution solved for the purge cycle differed somewhat from the RK solution because, in setting up the analytical solution, the RT term (ideal gas constant and MCO/Cask temperature) correlated to the total moles (from ideal gas law) in the Cask and MCO could be cancelled. However, in setting up the first order equations for the change in hydrogen gas fractions (both the Cask and MCO) with respect to time, for the RK solver, the total moles of gas in the Cask could not be cancelled (see attached calc derivations in Appendix A). Therefore, the RT term had to be retained, thus making the solution temperature dependent (it is assumed the temperature-dependent water/uranium reaction creating H₂ is constant at any MCO temperature). The RK method integrates with respect to time, whereas in the analytical solution the independent variable time t is substituted by the MCO pressure term derived from the overall mass balance.

[™] MATLAB is a registered trademark of The Mathworks, Inc.

i.e.,
$$n_1 = k\beta t + n_1^0 = \frac{PV_1}{RT} \quad \text{during the vent cycle}$$

or
$$P = \frac{RT}{V_1} (k\beta t + n_1^0)$$

And the change in pressure with time:

$$\frac{dP}{dt} = \frac{RTk\beta}{V_1} \quad \text{and} \quad P - P^0 = \frac{RTk\beta}{V_1} (t - t_0)$$

or
$$t - t_0 = \frac{V_1(P - P^0)}{RTk\beta}$$

Therefore, the time range required for each vent cycle RK solver step is:

$$\Delta t = \frac{V_1 \Delta P}{RTk\beta}$$

where: $\Delta t = t_{j+1} - t_j$ and $\Delta P = P_{j+1} - P_j$

Pressure increments of 0.1 psi were used in the analytical solution, so the same pressure increments were used in solving for the hydrogen fraction, with the above equation used for correlating the numerical solver time range per pressure increment.

The same time/pressure correlation is used for the purge cycle (for the numerical RK method) only α is used in the place of β .

$k = V_1/V_2$ V_1 = volume of Cask void space

V_2 = volume of MCO void space

P^0 = initial pressure (constant for each cycle)

P = MCO/Cask pressure (changing)

n_1^0 = initial mole gas in Cask

$$\beta = \frac{(n_{H2} - n_{Ex})}{(k+1)} = \frac{(n_{H2} - (2n_{H2} + n_{He}))}{(k+1)} = \frac{-(n_{H2} + n_{He})}{(k+1)}$$

$$\alpha = \frac{(n_{H2} + n_{He})}{(k+1)}$$

$$n_{H2} = \frac{\text{moles } H_2}{\text{min}} \quad n_{Ex} = \frac{\text{moles exhaust gas}}{\text{min}} \quad n_{He} = \frac{\text{moles He}}{\text{min}}$$

Therefore, this same correlation between pressure and time must be utilized in the RK routine when determining the integration time range with pressure change. In other words, if the Cask void space hydrogen fraction, y_1 , is being determined at P_{j+1} , an integration time range needs to be correlated between P_j and P_{j+1} . This is easily solved using the above linear time/pressure correlation.

1.5 Computer Model

See Section 1.4 for modeling application and EDT 626803 for MATLAB plotting routines and Runge-Kutta subroutine.

1.6 Input Data

High Nominal H_2 generation rate:	1.5×10^{-4} g H_2 /sec (Pajunen 1998)
"Best Estimate" High Nominal H_2 generation rate:	5.7×10^{-6} g H_2 /sec (Section 1.7)
Helium ingress rate:	1.9 SCFM (Irwin et al 1999)
Effective MCO void space volume:	0.56 ft ³ (Pajunen and Klimper 1998)
Cask void space volume:	0.53 ft ³ (Pajunen and Klimper 1998)
MCO and Cask water and void space temperature:	50°F (10°C) (Pajunen and Klimper 1998)

The Standard Conditions (SC) associated with the helium ingress rate is taken to be:

Temperature, $T = 0^\circ\text{C}$

Pressure, $P = 14.7$ psia

See Section 1.3 and EDT 626803 for input data.

1.7 Calculations

Six solutions are required overall for determining the hydrogen concentration in the Cask and MCO during the purge, delay, and vent cycles. These modeling equations are developed in Appendix A. Four analytical solutions were solved (Boyce and DiPrima 1969) for the H_2 concentration in the MCO and Cask during each purge and time delay cycle. An analytical solution was also determined for the H_2 concentration in the MCO during each vent cycle. A numerical method was used to determine the hydrogen concentration in the Cask during each vent cycle since an analytical solution was not apparent. The numerical solution utilizes a Runge-Kutta method for finding an approximate solution to the first order differential equation.

Solutions during Purge Cycle:

$$y_1 = y_1^0 (P^0/P)^{\gamma+1} \quad (P-1)$$

$$y_2 = k y_1^0 (P^0/P) [1 - (P^0/P)^{\gamma}] + y_2^0 (P^0/P) + (n_{H2}/\alpha) [1 - (P^0/P)] \quad (P-2)$$

where: y_1 = H₂ mole fraction in the Cask void space during the purge cycle
 y_1^0 = initial H₂ mole fraction in the Cask void space prior to purge cycle
 y_2 = H₂ mole fraction in the MCO void space during the purge cycle
 y_2^0 = initial H₂ mole fraction in the MCO void space prior to purge cycle
 P^0 = initial purge pressure at 15.2 psia (0.5 psig)
 P = purge pressure up to 35.2 psia (20.5 psig)
 V_1 = void space volume of the Cask
 V_2 = void space volume of the MCO
 k = ratio of the Cask and MCO void space volumes, V_1/V_2
 n_{He} = helium ingress rate, mole He/min
 n_{H2} = hydrogen generation rate, mole H₂/min
 α = $(n_{He} + n_{H2})/(k+1)$, mole/min
 γ = $(\alpha - n_{H2})/k\alpha$, dimensionless

Solutions during Delay Cycle after Purge:

$$y_1 = y_1^0 (P^0/P) + (k\alpha RT/PV_2) [(P^0/kP) y_2^0 t + (RT/2PV_1)(n_{H2} - k\alpha)t^2] \quad (D-1)$$

$$y_2 = (RT/PV_2) [y_2^0 n_2^0 + (n_{H2} - k\alpha)t] \quad (D-2)$$

where: y_1 = H₂ mole fraction in the Cask void space during the delay cycle
 y_1^0 = initial H₂ mole fraction in the Cask void space prior to the delay cycle
 y_2 = H₂ mole fraction in the MCO void space during the delay cycle
 y_2^0 = initial H₂ mole fraction in the MCO void space prior to the delay cycle
 R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
 T = MCO/Cask temperature, 283 K (10°C)
 n_2^0 = initial total moles in the MCO equal to $P^0 V_2 / RT$, mole
 P^0 = initial delay pressure at 35.2 psia
 P = delay pressure up to 35.3 psia during the two-minute delay
 t = time duration, minute

Solutions during Vent Cycle after Delay:

$$\frac{dy_1}{dt} = \frac{RT}{PV_1} [(n_{H2} - \beta)y_2 - (k\alpha + n_{Ex})y_1] \quad (V-1)$$

$$y_2 = (y_2^0 - 1)(P^0/P)^{\phi+1} + 1 \quad (V-2)$$

where: y_1 = H₂ mole fraction in the Cask void space during the vent cycle
 y_1^0 = initial H₂ mole fraction in the Cask void space prior to the vent cycle
 y_2 = H₂ mole fraction in the MCO void space during the vent cycle
 y_2^0 = initial H₂ mole fraction in the MCO void space prior to the vent cycle
 P^0 = initial vent pressure at 35.3 psia
 P = vent pressure down to 15.2 psia at the completion of the vent cycle
 n_{Ex} = helium exhaust rate, mole He/min
 β = $(n_{H2} - n_{Ex})/(k+1)$, mole/min
 ϕ = $(n_{H2} - \beta)/\beta$, dimensionless

To calculate the "best estimate" High Nominal hydrogen gas generation rate from Pajunen (1998):

Assume UH_3 does not react in liquid water

Reaction enhancement factor = 3 to account for roughness, etc.

$$R_H = A K (1/16) 10^{-3} \text{ mol H}_2/\text{hr}$$

$$= (47,000 \text{ cm}^2)(3.52 \times 10^{-3} \frac{\text{mg O}_2 \text{ wt gain}}{\text{cm}^2 \cdot \text{hr}})(\frac{1 \text{ mol H}_2}{16 \text{ g O}_2 \text{ wt gain}})(10^{-3} \frac{\text{g}}{\text{mg}})$$

$$= 0.0103 \frac{\text{mol H}_2}{\text{hr}}$$

$$= 1.72 \times 10^{-4} \frac{\text{mol H}_2}{\text{min}}$$

$$= 5.7 \times 10^{-6} \frac{\text{g H}_2}{\text{sec}}$$

1.8 Results

Results from Figure 1-1a, 1-1b, and 1-2 assume twenty continuous purge/vent cycles *without delay* between cycles. This operational scenario would be considered an ideal operation since the vent cycle would start immediately after the purge cycle with no delay time between cycles. Figure 1-1a shows the hydrogen concentration in the MCO and Cask over twenty cycles as a decrease of hydrogen with respect to time on a linear scale. Figure 1-1b shows the same input/output information as the previous plot but the hydrogen fraction is plotted on a semi-log scale to display easier-to-read results, especially in the latter cycles. From this plot, it can be shown that the Cask reaches approximately 1% H_2 after the 10-11th purge/vent cycle and the MCO is shown to be approximately 1.5% H_2 . Figure 1-2 shows the 20th purge/vent cycle hydrogen concentration in the MCO and Cask assuming continuous (no delay) operation. The hydrogen concentration is just below 1.2% in the MCO and just below 0.7% in the Cask.

Figures 1-3a, 1-3b, and 1-4 assume a two-minute delay only after each purge cycle. This is a more realistic scenario than the previous operation of no time delay since it will take some time for the pressure valves to be manually actuated with pressure being applied or vented. Note the two-minute delay is only after the purge cycle. A one-minute delay is actually assumed after each cycle but is combined and plotted only after the purge cycle since, numerically, both ways provide an equal solution over each complete cycle. Figure 1-3a shows the hydrogen concentration in the MCO and Cask void spaces over twenty cycles as a decrease of hydrogen with respect to time on a linear scale. Figure 1-3b shows the same input/output information as the previous plot but the hydrogen fraction is plotted on a semi-log scale. From this plot, it can be shown that the Cask reaches approximately 1.5% H_2 after the 10th purge/delay/vent cycle and the MCO is shown to be over 2% H_2 . The 20th cycle, with time delay can be better displayed in Figure 1-4. After venting, the Cask contains about 1.1% H_2 while the MCO contains just under

1.9% H₂. Note the increase in the hydrogen concentration in the MCO (where the hydrogen is being generated) after the purge cycle due to the two-minute delay between cycles.

Figure 1-6a shows the hydrogen concentration, using a “best estimate” High Nominal H₂ generation rate, in the MCO and Cask void spaces over twenty cycles as a decrease of hydrogen with respect to time on a linear scale. Figure 1-3b shows the same input/output information as the previous plot but the hydrogen fraction is plotted on a semi-log scale. From this plot, it can be shown that the MCO and Cask void spaces reach below 1% H₂ after the 10th purge/delay/vent cycle. The 20th cycle, with time delay can be better displayed in Figure 1-7. After venting, the Cask contains about 0.19% H₂ while the MCO contains just under 0.14% H₂. Note the increase in the hydrogen concentration in the MCO (where the hydrogen is being generated) after the purge cycle due to the two-minute delay between cycles.

Figures 1-8a, 1-8b, 1-9a, and 1-10b show the transient hydrogen gas concentration increase over a delayed period when no purge and vent cycles are in operation. Assuming after n purge/vent cycles, with initial delay H₂ gas concentrations of 1% and 0.7% in the MCO and Cask, respectively, transient H₂ concentrations are developed in these void spaces during a delay time up to 24 hours. Both High Nominal and “best estimate” High Nominal rates are included in this operation delay assumption.

1.9 Conclusions

Given the input parameters, the plots demonstrate, even under the ideal condition of non-stop (no time delay) purge/vent cycles using the High Nominal H₂ generation rate, that the 1% hydrogen concentration limit in both the MCO and Cask cannot be met. The more realistic approach using a 2-minute time delay after the purge cycle demonstrates that the MCO void space hydrogen concentration is clearly above the 1% limit. However, using the “best estimate” High Nominal H₂ generation rate, the 1% hydrogen gas limit can easily be met after 10 purge/delay/vent cycles.

1.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Pajunen, A. L. and Klimper, S. C., 1998, *Inert Gas Requirements For Cask Loading*, HNF-2833, Rev. 0, COGEMA Engineering Corporation, Richland, Washington.

Figure 1-1a MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During “No Delay Time” Helium Purge And Vent Cycle On Linear Scale

Figure 1-1b MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During “No Delay Time” Helium Purge And Vent Cycle On Semi-Log Scale

Figure 1-2 MCO And Cask Void Space Hydrogen (H_2) Concentration During 20th “No Delay Time” Helium Purge And Vent Cycle On Linear Scale

Figure 1-3a MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During “2-Minute Delay Time” After Helium Purge Followed By Vent Cycle On Linear Scale

Figure 1-3b MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During “2-Minute Delay Time” After Helium Purge Followed By Vent Cycle On Semi-Log Scale

Figure 1-4 MCO And Cask Void Space Hydrogen (H_2) Concentration During 20th “2-Minute Delay Time” Helium Purge Followed By Vent Cycle On Linear Scale

Figure 1-5 Numerical And Analytical Solution Comparison In The MCO (Y₂) And Cask (Y₁) During 20th “No Delay Time” Helium Purge Followed By Vent Cycle On Linear Scale

Figure 1-6a MCO And Cask Void Space Transient Hydrogen Gas (H₂) Concentration During “2-Minute Delay Time” After Helium Purge Followed By Vent Cycle On Linear Scale

Figure 1-6b MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During “2-Minute Delay Time” After Helium Purge Followed By Vent Cycle On Semi-Log Scale

Figure 1-7 MCO And Cask Void Space Hydrogen (H_2) Concentration During 20th “2-Minute Time” Helium Purge Followed By Vent Cycle On Linear Scale

Figure 1-8a MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During Delay After N^{th} Purge/Vent Cycle On Linear Scale Over 60 Minutes

Figure 1-8b MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During Delay After N^{th} Purge/Vent Cycle On Semi-Log Scale Over 60 Minutes

Figure 1-9a MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During Delay After N^{th} Purge/Vent Cycle On Linear Scale Over 24 Hours

Figure 1-9b MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During Delay After N^{th} Purge/Vent Cycle On Semi-Log Scale Over 24 Hours

Figure 1-10a MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During Delay After N^{th} Purge/Vent Cycle On Linear Scale Over 24 Hours W/ "Best Estimate" High Nominal H_2 Rate

Figure 1-10b MCO And Cask Void Space Transient Hydrogen Gas (H_2) Concentration During Delay After N^{th} Purge/Vent Cycle On Semi-Log Scale Over 24 Hours W/ "Best Estimate" High Nominal H_2 Rate.

2.0 Evaluation of MCO Void Gas Composition Prior to Draining

2.1 Purpose and Objectives

The purpose of this calculation is to ensure the helium purge and vent design basis is adequate for reducing hydrogen gas in the MCO void space after Cask removal and prior to MCO bulk water drain. A number of automated purge/vent cycles, with a time delay after the purge cycle, are to be determined, using conservative set pressure changes (4 psig to 1 psig), to reduce the hydrogen gas concentration below 1% (mole H₂/mole total gas) in the void space.

2.2 Summary of Final Results and Conclusions

An overall mass (mole) and hydrogen balance was performed around the MCO void space volume. Analytical solutions were reached for hydrogen mole fractions for the purge, delay, and vent cycles (Boyce and DiPrima 1969). Various time delays (2 minute, 1 minute, 30 seconds, 15 seconds, and 5 seconds for High Nominal hydrogen generation rates), after each purge cycle, are included with resulting plots (Figure 1-1 through 1-5) to show the hydrogen concentration in the MCO void space. Two plots (Figure 1-6 and 1-7) include time delays of 15 and 5 seconds after the purge cycle to show the hydrogen concentration change using the Bounding hydrogen generation rate.

Based on a High Nominal hydrogen generation rate and a 2.5 second valve actuation delay, a pressure cycle of 1 to 4 psig cannot achieve a steady state hydrogen concentration below 1.2%. The pressure change must be increased somewhat above 4 psig in order to ensure the hydrogen remains below 1% in the MCO void space during High Nominal hydrogen generation.

Based on a Bounding hydrogen generation rate and a 2.5 second valve actuation delay, a pressure cycle of 1 to 4 psig cannot achieve a steady state hydrogen concentration below 4.5%. The pressure change must be increased somewhat above 4 psig in order to ensure the hydrogen remains below 1% in the MCO void space during Bounding hydrogen generation.

2.3 Assumptions

The helium flow rate is assumed to be 150 SCFM. The hydrogen generation rate used is the high nominal value of 6.4×10^{-4} g/sec and the bounding value is 2.4×10^{-3} g/sec (Pajunen 1998). Helium gas (assumed 100% He) is used to purge the MCO from 1 psig (15.7 psia) to 4 psig (18.7 psia). The helium purge is assumed to instantly mix with the MCO void space gas. No piping volume carrying the helium to the MCO void space is included. The initial hydrogen mole fraction is conservatively assumed to be 0.998. The MCO gas temperature is taken to be 50°C with MCO water assumed to be hydrogen saturated.

Time delay durations are used for comparative sensitivity with the H_2 increase in the MCO void space over delay time. The time delays are taken after the purge cycle to represent valve operation delay between the purge and vent cycles. Each delay duration represents the total valve actuation delay time taken over one cycle. One cycle consists of one purge, delay, and vent cycle. Five different time delay durations are assumed after the purge cycle for the high nominal value. They consist of a 2-minute, 1-minute, 30-second, 15-second, and 5-second duration. Two different time delay durations are assumed after the purge cycle for the bounding value. They consist of a 15-second and 5-second duration.

2.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626803).

2.5 Computer Model

Not applicable to this calculation.

2.6 Input Data

High Nominal H_2 generation rate:	6.4×10^{-4} g H_2 /sec (Pajunen 1998)
Bounding H_2 generation rate:	2.4×10^{-3} g H_2 /sec (Pajunen 1998)
Helium ingress rate:	150 SCFM (Section 2.3)
Effective MCO void space volume:	0.56 ft ³ (Pajunen and Klimper 1998)
MCO water and void space temperature:	50°C (Irwin et al 1999)

The Standard Conditions (SC) associated with the helium ingress rate is taken to be:

Temperature, $T = 0^\circ\text{C}$

Pressure, $P = 14.7$ psia

See Section 2.3 and EDT 626803 for input data.

2.7 Calculations

Three solutions are required overall for determining the hydrogen concentration in the MCO during the purge, delay, and vent cycles. These modeling equations are developed in Appendix B.

Solution during the Purge Cycle:

$$y = (P^0/P) \left[y^0 - (n_{H_2}/\alpha) \right] + (n_{H_2}/\alpha) \quad (P-1)$$

where: y = H_2 mole fraction in the MCO void space during the purge cycle
 y^0 = initial H_2 mole fraction in the MCO void space prior to purge cycle
 P^0 = initial purge pressure at 15.7 psia (1 psig)
 P = purge pressure up to 18.7 psia (4 psig)
 n_{He} = helium ingress rate, mole He/min
 n_{H_2} = hydrogen generation rate, mole H_2 /min
 α = $(n_{He} + n_{H_2})$, mole/min

Solution during the Delay Cycle: (D-1)

$$y = (P^0/P)(y^0 - 1) + 1$$

where: y = H_2 mole fraction in the MCO void space during the delay cycle
 y^0 = initial H_2 mole fraction in the MCO void space prior to delay cycle
 P^0 = initial time delay cycle pressure in the MCO void space at 18.7 psia (4 psig)
 P = the time delay pressure in the MCO void space pressure

Solution during the Vent Cycle after Purge:

$$y = 1 + (y^0 - 1)(P^0/P)^{\gamma+1} \quad (V-1)$$

where: y = H_2 mole fraction in the MCO void space during the vent cycle
 y^0 = initial H_2 mole fraction in the MCO void space prior to the vent cycle
 P^0 = initial vent pressure in the MCO void space at 18.7 psia (4 psig)
 P = vent pressure in the MCO void space down to 15.7 psia (1 psig) during the vent cycle
 β = $(n_{H_2} - n_{Ex})$, mole/min
 γ = n_{Ex}/β , dimensionless

2.8 Results

The more realistic input includes delay times of 1 or 2 minutes during each cycle. Using High Nominal hydrogen generation rates, the H_2 percentage in the MCO void space lies well above 10% for the 1 minute delay (Figure 2-2) and above 20% for the 2 minute delay (Figure 2-1). If the delay time takes only 15 to 30 seconds over each cycle, the H_2 percentage is reduced to 4 - 7%. Assuming both purge and vent valves can quickly actuate from a close-to-open (and visa versa) position over a total 5 seconds (2.5 seconds each), with a High Nominal hydrogen generation rate, Figure 2-5 shows the 1% H_2 can not quite be reached.

Two plots using the Bounding hydrogen generation rate are included to show that the "best case" scenario (5 - 15 second total cycle delay) under bounding conditions results in a H_2 percentage in the MCO void space of 4.5 - 13%.

2.9 Conclusions

Given the input parameters, the plots demonstrate the transient hydrogen concentration in the MCO cannot realistically reach the 1% limit.

2.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Pajunen, A. L. and Klimper, S. C., 1998, *Inert Gas Requirements For Cask Loading*, HNF-2833, Rev. 0, COGEMA Engineering Corporation, Richland, Washington.

Figure 2-1 MCO Void Space Transient Hydrogen Gas (H₂) Concentration During "2-Minute Delay Time" Helium Purge And Vent Cycle On Semi-Log Scale. High Nominal H₂ Generation Rate

Figure 2-2 MCO Void Space Transient Hydrogen Gas (H₂) Concentration During "1-Minute Delay Time" Helium Purge And Vent Cycle On Semi-Log Scale. High Nominal H₂ Generation Rate

Figure 2-3 MCO Void Space Transient Hydrogen Gas (H₂) Concentration During "30-Second Delay Time" Helium Purge And Vent Cycle On Semi-Log Scale. High Nominal H₂ Generation Rate

Figure 2-4 MCO Void Space Transient Hydrogen Gas (H₂) Concentration During "15-Second Delay Time" Helium Purge And Vent Cycle On Semi-Log Scale. High Nominal H₂ Generation Rate

Figure 2-5 MCO Void Space Transient Hydrogen Gas (H_2) Concentration During "5-Second Delay Time" Helium Purge And Vent Cycle On Semi-Log Scale. High Nominal H_2 Generation Rate

Figure 2-6 MCO Void Space Transient Hydrogen Gas (H_2) Concentration During "15-Second Delay Time" Helium Purge And Vent Cycle On Semi-Log Scale. Bounding H_2 Generation Rate.

Figure 2-7 MCO Void Space Transient Hydrogen Gas (H_2) Concentration During "5-Second Delay Time" Helium Purge And Vent Cycle On Semi-Log Scale. Bounding H_2 Generation Rate

3.0 Evaluation of Helium Pre-Purge to Reduce Oxygen Concentrations in the PWC Receiving Tanks

3.1 Purpose and Objectives

The purpose of this calculation is to ensure the design basis is adequate for reducing oxygen gas concentrations in the PWC Receiving Tanks (PWC-TK-4032 and PWC-TK-4033) prior to the MCO bulk water drain. The helium purge time to reduce the oxygen concentration below 1.6% (or 0.016 mole O₂/mole total gas) in both PWC tanks is required.

3.2 Summary of Final Results and Conclusions

An overall mass (mole) and helium balance was performed around the PWC Receiving Tanks (mathematical derivations attached in Appendix C). An analytical solution was reached for the helium mole fraction (and, thus, the oxygen mole fraction) in both PWC Receiving Tank void spaces as a function of helium purge time (Boyce and DiPrima 1969). Figure 3-1 shows it takes approximately 6 minutes and approximately 9.5 minutes to reach the 1.6% O₂ level in PWC-TK-4032 (Tank 1) and PWC-TK-4033 (Tank 2), respectively.

3.3 Assumptions

This problem is analyzed as a two-component system – helium and air. The oxygen concentration is estimated assuming the composition of air remains constant while purged with helium. Helium gas (assumed 100% He) is used to purge the PWC tanks which are continually vented at 1 atm. The helium flow rate into the PWC tanks is 8 SCFM. The tank void spaces are assumed to be connected in series while the gases in both tanks are assumed to be well-mixed. The initial oxygen mole fraction is assumed to be 0.21 mole/mole gas; in other words, the PWC tank void spaces (both receiving tanks) are assumed to initially contain air.

PWC Receiving Tank 1 void space (tank assumed empty of water) consists of approximately 160gal (20 ft³) and Tank 2 void space consists of 125 gal (16.7 ft³) or 175 gal (empty) minus 50 gal water minimum for pumping = 125 gal. Perfect gas mixing in both tanks assumed. Piping volume to and from both tanks is assumed to be negligible. The temperature in the PWC tanks is assumed to be 10°C.

3.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626803).

3.5 Computer Model

Not applicable to this calculation.

3.6 Input Data

Helium ingress rate: 8 SCFM (Irwin et al 1999)
 PWC Tank 1 void volume: 20 ft³ (H-1-82164, Rev. 1)
 PWC Tank 2 void volume: 16.7 ft³ (Section 3.3)
 PWC tanks temperature: 10°C (Section 3.3)

The Standard Conditions (SC) associated with the helium ingress rate is taken to be:
 Temperature, $T = 0^{\circ}\text{C}$
 Pressure, $P = 14.7 \text{ psia}$

See Section 3.3 and EDT 626803 for input data.

3.7 Calculations

Two solutions are required overall for determining the hydrogen concentration in the PWC tanks during the helium purge. These modeling equations are developed in Appendix C

Solution in PWC Tank 1:

$$y_1 = (y_1^0 - 1)e^{\gamma t} + 1 \quad (\text{P-1})$$

where: y_1 = helium mole fraction in PWC Tank 1 void space
 y_1^0 = initial helium mole fraction in PWC Tank 1 void space
 n_{He} = the helium ingress rate, mole He/min
 $P = 1 \text{ atm}$
 $R = \text{ideal gas constant, } 0.04259 \text{ (psia-ft}^3\text{)/(mole-K)}$
 $T = \text{MCO/Cask temperature, } 294 \text{ K (21}^{\circ}\text{C)}$
 $V_1 = \text{void space volume of PWC Tank 1}$
 $n_1 = \text{total moles in PWC Tank 1 void space equal to } PV_1/RT, \text{ mole}$
 $\gamma = n_{He}/n_1, \text{ min}^{-1}$
 $t = \text{helium purge time, min}$

The oxygen fraction, $[O_2]$, in PWC Tank 1 is therefore equal to $0.21(1 - y_1)$.

Solution in PWC Tank 2:

$$y_2 = [(y_2^0 - 1) + \beta]e^{-\phi t} - \beta e^{-\gamma t} + 1 \quad (\text{P-2})$$

where: y_2 = helium mole fraction in PWC Tank 2 void space
 y_2^0 = initial helium mole fraction in PWC Tank 2 void space
 n_{Ex} = gas exhaust rate, mole/min
 n_2 = initial total moles in PWC Tank 2 void space, mole
 $\beta = \frac{n_1(1 - y_1^0)}{(n_1 - n_2)}$, dimensionless
 $\phi = n_{Ex}/n_2, \text{ min}^{-1}$

The oxygen fraction, $[O_2]$, in PWC Tank 2 is therefore equal to $0.21(1 - y_2)$.

3.8 Results

Figure 3-1 uses the bounding initial value of 21% oxygen in both tanks, assuming air has filled both tanks. This plot shows Tank 1, where purge is initiated, takes approximately 6 minutes to reduce the O₂ concentration to 1.6%. Tank 2, connected in series to Tank 1, is shown to take less than 10 minutes to meet the same O₂ concentration.

3.9 Conclusions

Given the input parameters, the plot demonstrates that the oxygen concentration limit of 1.6% can be reached in both PWC Receiving Tanks within 10 ten minutes after start of helium purge.

3.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Figure 3-1 PWC Receiving Tanks Void Space Transient Oxygen (O_2) Concentration During Helium Purge On Linear Scale

4.0 Evaluation of PWC Receiving Tanks Void Gas Composition During Pre-Purge Delay

4.1 Purpose and Objectives

The purpose of this calculation is to ensure the design basis is adequate for reducing oxygen gas concentrations in the PWC Receiving Tanks, PWC-TK-4032 (Tank 1) and PWC-TK-4033 (Tank 2), prior to the MCO bulk water drain. The time to reduce the oxygen concentration below 1.6% (or 0.016 mole O₂/mole total gas) in both PWC tanks is required.

4.2 Summary of Results and Conclusions

Air ingress is caused by molecular diffusion, immediately following the helium purge, from the 1-inch diameter transfer piping from tank PWC-TK-4001 to Tank 2. An overall mass (mole) and air balance was performed around Tank 2 (mathematical derivations in Appendix D).

An analytical solution was reached for the air mole fraction in the Tank 2 void space as a function of air ingress time immediately after the helium purge (Boyce and DiPrima 1969). Figure 4-1 shows that it takes about 4 days to reach the 1.6% O₂ level in the PWC tank void space, conservatively assumed to be disconnected to Tank 1 with minimal pipe length, conservatively assumed 1 ft, from air source, PWC-TK-4001, to Tank 2. In Figure 4-2, the air source pipe length is conservatively assumed to be 10 ft in length, which shows it takes less than 40 days to reach the 1.6% O₂ level in the PWC tank void space.

4.3 Assumptions

This molecular diffusion analysis is treated as a pseudo-steady state equimolar counterdiffusion analysis. Also, it is assumed the air diffuses into only the closest tank (Tank 2), being further conservative by neglecting the entire pipe length ($z = 1$ ft and 10 ft) from the air source (PWC-TK-4001). This greatly simplifies this problem, while being conservative, since the additional connected tank, Tank 1, would only further dilute the ingress air (oxygen) and the added pipe length would only cause an increase in time delay to reach 1.6% O₂ in the PWC tank(s).

The initial air concentration in the PWC tank is 0%, which assumes the previous PWC Receiving Tanks helium purge brought the oxygen concentration down to 0% in both tanks. The initial time is taken to be immediately after the helium purge. The PWC tank void space is assumed to be 125 gal (16.7 ft³) (or 175 gal (empty) minus 50 gal water minimum for pumping = 125 gal). Perfect gas mixing in the tank is assumed. Air is assumed to consist of a constant 21% O₂.

4.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solution (see EDT 626803).

4.5 Computer Model

Not applicable to this calculation.

4.6 Input Data

PWC Tank 1 void volume: 20 ft³ (H-1-82164, Rev. 1)

PWC Tank 2 void volume: 16.7 ft³ (Section 4.3)

See Sections 4.3 and 4.7, and EDT 626803 for input data.

4.7 Calculations

One solution is required for determining the oxygen concentration in PWC Tank 2 during the delay. This modeling equation is developed in Appendix D.

Solution in Tank 2 :

$$y = 1 - e^{-\alpha t} \quad (D-1)$$

where: y = air mole fraction in the PWC tank void space
 $\mathcal{D}_{AB}$ = diffusion coefficient, equal to $\frac{10^3 T^{1.75} [(M_A + M_B)/M_A M_B]^{1/2}}{P[(\Sigma)_A^{1/3} + (\Sigma)_B^{1/3}]^2}$, cm²/sec
 M_A = molecular weight of A (taken here as air), 29 g/mole
 M_B = molecular weight of B (taken here as helium), 4 g/mole
 z = length of the air ingress piping, conservatively assumed to be 1 ft and 10 ft
 A = cross-sectional area of the air ingress piping, ft²
 P = 1 atm
 T = ambient temperature, 294 K (21°C)
 V = void space volume of the PWC tank
 $(\Sigma)_A$ = atomic diffusion volume for air taken from Perry's 6th Ed., Table 3-342
 $(\Sigma)_B$ = atomic diffusion volume for helium taken from Perry's 6th Ed., Table 3-342
 $\alpha = \frac{\mathcal{D}_{AB} A}{z V}$, hr⁻¹ (where $\mathcal{D}_{AB}$ is equal to 3600($\mathcal{D}_{AB}$))
 t = diffusion time, hr

The oxygen fraction, [O₂], in Tank 2 is therefore equal to 0.21y.

4.8 Results

Figure 4-1 shows the O₂ concentration in Tank 2 would reach 1.6% under the most conservative conditions. It assumes there is no connected Tank 1 to help dilute the oxygen. More importantly, it assumes minimal ingress piping length (only 1 ft), whereas in Figure 4-2, a more realistic length (but still conservative) of 10 ft is used. Using this still conservative length of ingress piping results in a time duration of almost 40 days before the oxygen concentration in Tank 2 reaches 1.6%.

4.9 Conclusions

Given the input parameters, the plots demonstrate that the oxygen concentration in both tanks, conservatively represented here with just one tank and short air ingress piping, will take well over a month to reach the 1.6% oxygen limit.

4.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Perry, R. H., and D. W. Green, 1984, *Perry's Chemical Engineer's Handbook, Sixth Edition*, M^CGraw-Hill Book Company, New York, New York.

Figure 4-1 PWC-TK-4033 Void Space Oxygen (O_2) Concentration During Air Leakage From 1-Inch Pipe Connected To Air Source. Assumes 1-Inch Diameter Air Ingress Pipe Is 1 Ft In Length

Figure 4-2 PWC-TK-4033 Void Space Oxygen (O_2) Concentration During Air Leakage From 1-Inch Pipe Connected To Air Source. Assumes 1-Inch Diameter Air Ingress Pipe Is 10 Ft In Length

5.0 Evaluation of PWC Receiving Tanks Void Gas Composition Following MCO Bulk Water Drain

5.1 Purpose and Objectives

The purpose of this calculation is to ensure the design basis is adequate for determining oxygen concentrations in the void space of the PWC Receiving Tanks, PWC-TK-4032 (Tank 1) and PWC-TK-4033 (Tank 2), following the MCO bulk water drain. Once the MCO bulk water drain is complete, oxygen ingress from PWC storage tank TK-4001 into the PWC Receiving Tanks, is initiated by the cooling down of the heated MCO bulk drain water. The time which the oxygen concentration remains below 1.6% (or 0.016 mole O₂/mole total gas) in both PWC tanks is required.

5.2 Summary of Results and Conclusions

An energy balance (actually, a thermal equilibrium or heat balance, since all energy is assumed to be in the form of heat) was performed around the system, taken to be the water in each PWC tank (McCabe, Smith, and Harriott 1993). Ingress air is transferred via bulk flow as the gas inside the PWC tanks loses heat.

Analytical solutions were reached for the air (21% oxygen) mole fractions in the void space of the PWC tanks (Boyce and DiPrima 1969). Table 5-1 summarizes the values from the solution for both tanks at two different time durations, 8 hrs and 24 hrs.

Based on the input parameters, the oxygen concentration reaches 1.5% in PWC Tank 2 (closest to air source) in approximately 8 hours after MCO bulk water drain.

Table 5-1

Tank Volume of 120 gal after 8 hours	PWC Tank 1	PWC Tank 2
Oxygen (mole/mole gas)	3.0 x 10 ⁻⁴	0.015
Tank Temperature (°F)	98	98
Tank Volume of 120 gal after 24 hours	PWC Tank 1	PWC Tank 2
Oxygen (mole/mole gas)	1.0 x 10 ⁻³	0.027
Tank Temperature (°F)	78	78

5.3 Assumptions

The water in the PWC tanks is continually circulated but the water is assumed to lose no heat through the transfer piping; therefore, the water in each tank is assumed to be well-mixed with no temperature gradients. Heat transfer is only taken at the water/tank wall boundary. No heat transfer is taken at the void space/tank wall boundary or mixing of ingress air. The tank void space temperature (both tanks) is assumed to be equal to the water temperature. The heat capacity of water from 70-122°F is assumed constant.

An overall mass (mole) and air balance was performed around the two PWC Receiving Tanks. Since the pressure in each tank is assumed to remain constant (1 atm) the moles of gas in the tank must increase (from ingress air) as the tank temperature decreases. No molecular or thermal diffusion is accounted for during air ingress. Heated drain water from the MCO, initially at 50°C (122°F), is transferred to the PWC Tanks. The ambient air temperature surrounding the PWC tanks is assumed to be 21°C (70°F).

A representative case is run which includes the volume of water in each tank at the time of the delay. This assumes each tank contains approximately 120 gal of water (5 vertical ft of cylindrical tank plus bottom conical section). The volume of water in each tank is assumed to be equal (the water being continually circulated) but the void volumes are different due to the different empty (or total) tank volumes. Initial oxygen concentrations in both tanks are assumed to be zero after helium purge. The delay time is run out to eight hours. Figures are also shown with delay time extended to 24 hours.

5.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626803).

5.5 Computer Model

Not applicable to this calculation.

5.6 Input Data

Initial temperature of water in PWC tanks:	50°C (Irwin et al 1999)
Ambient temperature outside of PWC tanks:	21°C (Section 5.3)
Volume of water in each PWC tank:	120 gal (Section 5.3)
Initial O ₂ concentration in both PWC tanks:	0% (Section 5.3)

See Section 5.3 and 5.7 and EDT 626803 for input data.

5.7 Calculations

Three solutions are required overall for determining the air (and, thus, oxygen) concentration in the PWC tanks during the delay after the MCO bulk water transfer. These modeling equations are developed in Appendix E. Temperature in PWC tanks as a function of time:

$$T = e^{-\beta t} (T^0 - c/\beta b) + c/\beta b \quad (T-1)$$

where: T = temperature of the water/gas in the PWC tanks, °F
 T^0 = temperature of the water/gas in the PWC tanks, °F
 T_{air} = temperature of the ambient air, °F
 h_1 = water film heat transfer coefficient (inside tank), 345 Btu/(ft²-hr-°F)
 h_2 = air heat transfer coefficient (outside tank) 2.18 Btu/(ft²-hr-°F) (McCabe, Smith, and Harriott 1993)
 l = PWC tank wall thickness, ft
 A = area of heat transfer area, ft²
 m = mass water in each tank, lb_m
 C_p = heat capacity of water at 70-122°F, 1 Btu/lb_m-°F
 k = thermal conductivity of steel, 26 Btu/(ft-hr-°F) (McCabe, Smith, and Harriott 1993)
 $\beta = \frac{h_2 A}{m C_p} \text{ hr}^{-1}$
 $a = \frac{T_{air}(h_2 + h_1 h_2 l/k)}{(h_1 + h_2 + h_1 h_2 l/k)}, \text{ °F}$
 $b = \frac{h_1}{(h_1 + h_2 + h_1 h_2 l/k)}, \text{ dimensionless}$
 $c = \beta(T_{air} - a), \text{ °F/hr}$

Solution in Tank 1:

$$y_1 = (T/T^0) [1 - (T/T^0)^k] (y_2^0 - 1) + (T/T^0) (y_1^0 - 1) + 1 \quad (D-1)$$

where: y_1 = air mole fraction in the PWC Tank 1 void space during cooling
 y_1^0 = initial air mole fraction in the PWC Tank 1 void space
 y_2^0 = initial air mole fraction in the PWC Tank 2 void space
 V_1 = void space volume of PWC Tank 1, ft³
 V_2 = void space volume of PWC Tank 2, ft³
 k = ratio of the PWC tanks void space volumes, V_1/V_2
 T = temperature of the PWC tanks, K
 T^0 = initial temperature of the PWC tanks, K

The oxygen fraction, y_{O_2} , in PWC Tank 1, is therefore equal to $0.21y_1$.

Solution in Tank 2:

$$y_2 = (T/T^0)^{1+k} (y_2^0 - 1) + 1 \quad (D-2)$$

where: y_2 = air mole fraction in the PWC Tank 2 void space during cooling
 y_2^0 = initial air mole fraction in the PWC Tank 2 void space

The oxygen fraction, y_{O_2} , in PWC Tank 2, is therefore equal to $0.21y_2$.

5.8 Results

The first two plots show the results of approximately 120 gal of water in each tank up to 8 hours delay time. Figure 5-1 shows the increase in the oxygen concentration in both PWC tanks as a function of delay time. This plot shows the oxygen concentration approximately reaches 1.6% after 8 hours delay time. Figure 5-2 shows the increase in the oxygen concentration in both PWC tanks as the tank temperature decreases. The oxygen mole fraction is plotted on semi-log in both plots. The last two figures display the same parameters as the previous two except the delay time is up to 24 hours.

5.9 Conclusions

Given the input parameters, the plots demonstrate that the oxygen concentration in Tank 2 will take approximately 8 hours, beginning immediately after the MCO bulk water drain and following helium purge, to reach the 1.6% oxygen limit.

5.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

McCabe, W. L., J. C. Smith, and P. Harriott, 1993, *Unit Operations of Chemical Engineering, Fifth Edition*, M^cGraw-Hill Book Company, New York, New York.

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Figure 5-1 PWC Receiving Tanks Void Space Transient Oxygen (O_2) Concentration During Time Delay “Cool Down” Period After MCO Bulk Water Drain On Semi-Log Scale Over 8 Hours

Figure 5-2 PWC Receiving Tanks Void Space Oxygen (O_2) Concentration During “Cool Down” Period After MCO Bulk Water Drain On Semi-Log Scale Over 8-Hour Period

Figure 5-3 PWC Receiving Tanks Void Space Transient Oxygen (O_2) Concentration During Time Delay “Cool Down” Period After MCO Bulk Water Drain On Semi-Log Scale Over 24 Hours

Figure 5-4 PWC Receiving Tanks Void Space Oxygen (O_2) Concentration During “Cool Down” Period After MCO Bulk Water Drain On Semi-Log Scale Over 24-Hour Period

6.0 Evaluation of Helium Purge to Reduce Hydrogen Gas Concentrations in the PWC Receiving Tanks Void Space Following MCO Bulk Water Drain

6.1 Purpose and Objectives

The purpose of this calculation is to ensure the helium purge design basis is adequate for reducing hydrogen gas concentrations in the PWC Receiving Tanks, PWC-TK-4032 (Tank 1) and PWC-TK-4033 (Tank 2), following the MCO bulk water drain. The time which the hydrogen concentration is reduced below 1% (0.01 mole H_2 /mole total gas) in both PWC tanks is required.

6.2 Summary of Results and Conclusions

The hydrogen gas generated (for both high nominal and bounding) in the MCO during the drain cycle of 45 minutes is transferred (purged) to the two PWC Receiving Tanks. An overall mass (mole) and helium balance was performed around the PWC tanks. The initial moles of hydrogen in each tank (assumed equal concentrations) were calculated by multiplying the hydrogen generation rate (both high nominal and bounding) by the delay time of 45 minutes. Analytical solutions were reached for the helium mole fractions in the void spaces of both PWC tanks with the H_2 mole fraction calculated (i.e., $1 - y_{He}$) for each tank (Boyce and DiPrima 1969).

Based on the conservative Bounding hydrogen generation rate, the hydrogen concentration in both PWC tanks is reduced below 1% with a helium purge time of 3.2 minutes at 8 SCFM.

6.3 Assumptions

Perfect mixing of the total hydrogen gas generated in the MCO is assumed in both PWC tanks with the initial (before PWC post helium purge) concentration equal in both tanks as well. Pressure in both tanks is taken at 1 atm. Both tanks are assumed to only contain hydrogen and helium. The purge helium volumetric flow rate is 8 SCFM. Temperature in the PWC tanks assumes the recently purged gas is at 50°C. The nominal case of 230 gal of water (150 gal MCO bulk water drain plus 80 gal flush water) is assumed which is transferred to the PWC tanks in equal volumes (115 gal each tank). However, a case is run for both high nominal and bounding when the PWC tanks possess equal void space volumes.

The initial hydrogen concentrations are calculated at 6% and approximately 18% for the high nominal and bounding cases, respectively. These initial values were calculated from the nominal case of 115 gal water in each PWC tank with the remaining unequal void spaces in the PWC tanks containing the purge hydrogen gas from the MCO (Tank 1 void volume = $(160 - 115)$ gal = 45 gal or 6 ft³ and Tank 2 void volume = $(175 - 115)$ gal = 60 gal or 8 ft³).

6.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626803).

6.5 Computer Model

Not applicable to calculation.

6.6 Input Data

High Nominal (HN) H ₂ generation rate:	6.4×10^{-4} g H ₂ /sec (Pajunen 1998)
Bounding (B) H ₂ generation rate:	2.4×10^{-3} g H ₂ /sec (Pajunen 1998)
Helium ingress rate:	8 SCFM (Irwin et al 1999)
For unequal PWC tank void space volumes:	
PWC Tank 1:	6 ft ³ (Section 6.3)
PWC Tank 2:	8 ft ³ (Section 6.3)
MCO bulk water and PWC void space temperature:	50°C (Irwin et al 1999)
Initial H ₂ concentration in PWC tanks w/HN H ₂ rate:	6% (Appendix F)
Initial H ₂ concentration in PWC tanks w/B H ₂ rate:	18% (Appendix F)

The Standard Conditions (SC) associated with the helium ingress rate is taken to be:

Temperature, T = 0°C

Pressure, P = 14.7 psia

See Section 6.3, Appendix F, and EDT 626803 for input data.

6.7 Calculations

Three solutions are required overall for determining the helium (and, thus, hydrogen) concentration in the Cask and MCO during the purge, delay, and vent cycles. These modeling equations are developed in Appendix F.

Solution in PWC Tank 1 (for both unequal and equal tank void volumes):

$$y_1 = (y_1^0 - 1)e^{-\gamma t} + 1 \quad (\text{P-1})$$

where:

- y_1 = helium mole fraction in the PWC Tank 1 void space during purge
- y_1^0 = initial helium mole fraction in the PWC Tank 1 void space
- n_{He} = helium ingress rate, mole He/min
- V_1 = void space volume of PWC Tank 1, ft³
- T = temperature of the PWC tanks, K
- R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
- P = atmospheric pressure, 14.7 psia
- n_1 = total moles of gas in PWC Tank 1 equal to PV_1/RT , mole
- $\gamma = n_{He}/n_1$, min⁻¹
- t = purge time, min

The hydrogen fraction, y_{H_2} , in PWC Tank 1, is therefore equal to $(1 - y_1)$.
Solution in PWC Tank 2 (for unequal tank void volumes):

$$y_2 = (y_2^0 - 1)e^{-\phi t} + \frac{\phi(y_1^0 - 1)}{(\phi - \gamma)}[e^{-\gamma t} - e^{-\phi t}] + 1 \quad (P-2)$$

where: y_2 = helium mole fraction in the PWC Tank 2 void space during purge
 y_2^0 = initial helium mole fraction in the PWC Tank 2 void space
 n_2 = total moles of gas in PWC Tank 2 equal to PV_2/RT , mole
 $\phi = n_{He}/n_2, \text{ min}^{-1}$

Solution in PWC Tank 2 (for equal tank void volumes):

$$y_2 = e^{-\gamma t}[(y_2^0 - 1) + \gamma(y_1^0 - 1)t] + 1 \quad (PE-2)$$

The hydrogen fraction, y_{H_2} , in PWC Tank 2 (for both unequal and equal tank void volumes), is therefore equal to $(1 - y_2)$.

6.8 Results

Figures 6-1 and 6-2 show the (high nominal case) H_2 concentration versus purge time for the PWC tanks on semi-log scale, assuming the PWC tank void volumes are unequal and equal, respectively. Figures 6-3 and 6-4 show the bounding case for both PWC tanks, assuming the PWC tank void volumes are unequal and equal, respectively. The longest purge time, judging from the plots, comes from PWC Tank 2, which can be easily purged of hydrogen ($< 1\%$), after approximately 190 seconds of helium purge, conservatively assuming the bounding case with the input helium purge rate at 8 SCFM.

6.9 Conclusions

Given the input parameters, the plots demonstrate that the helium purge duration will take approximately 3.2 minutes (190 seconds) to reach the 1% H_2 limit for both tanks, using the Bounding hydrogen gas generation rate.

6.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Figure 6-1 PWC Receiving Tanks Void Space (Unequal Volumes) Transient Hydrogen (H_2) Concentration During Helium Purge After MCO Bulk Water Drain On Semi-Log Scale

Figure 6-2 PWC Receiving Tanks Void Space (Equal Volumes) Transient Hydrogen (H_2) Concentration During Helium Purge After MCO Bulk Water Drain On Semi-Log Scale

Figure 6-3 PWC Receiving Tanks Void Space (Unequal Volumes) Transient Hydrogen (H_2) Concentration During Helium Purge After MCO Bulk Water Drain On Semi-Log Scale

Figure 6-4 PWC Receiving Tanks Void Space (Equal Volumes) Transient Hydrogen (H_2) Concentration During Helium Purge After MCO Bulk Water Drain On Semi-Log Scale

7.0 Evaluation of Helium Purge to Reduce Hydrogen Gas Concentrations in the MCO Void Space Prior to Entering Vacuum Mode

7.1 Purpose and Objectives

The purpose of this calculation is to ensure the helium purge design basis is adequate for reducing hydrogen gas in the MCO void space prior to entering vacuum mode. The total gas volume replacement is required by measuring the actual helium flow with a minimum flow of 8 SCFM. The hydrogen concentration needs to be reduced below 1% (0.01 mole H₂/mole total gas) in the MCO void space.

7.2 Summary of Final Results and Conclusions

An overall mass (mole) and hydrogen balance was performed around the MCO (mathematical derivations attached in Appendix G). An analytical solution was reached for the hydrogen mole fraction in the MCO void space (nominal 500 L) as a function of helium purge time (Boyce and DiPrima 1969).

Given the input parameters with the Bounding hydrogen generation rate, Figures 7-3 and 7-4 demonstrate that the helium purge duration will take approximately 12 minutes and 90 SCF helium to reach the 1% H₂ limit in the MCO void space, using the Bounding hydrogen gas generation rate.

7.3 Assumptions

The helium flow rate is 8 SCFM. The hydrogen generation rate is the high nominal value of 1.9×10^{-3} g/sec (0.057 mole/min) and the bounding value used is 2.4×10^{-3} g/sec. Helium gas (assumed 100% He) is used to purge the MCO which is vented and maintained at 1 psig. The MCO gas temperature is assumed to be 50°C. The initial hydrogen mole fraction is assumed to be 0.998 mole H₂/mole gas.

7.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626803).

7.5 Computer Model

Not applicable to calculation.

7.6 Input Data

High Nominal (HN) H ₂ generation rate:	1.9 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
Bounding (B) H ₂ generation rate:	2.4 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
Helium ingress rate:	8 SCFM (Irwin et al 1999)
MCO water and void space temperature:	50°C (Irwin et al 1999)
MCO void space pressure:	1 psig (Section 7.3)

The Standard Conditions (SC) associated with the helium ingress rate is taken to be:

Temperature, T = 0°C

Pressure, P = 14.7 psia

See Section 7.3 and EDT 626803 for input data.

7.7 Calculations

One solution is required for determining the hydrogen concentration in the MCO during the helium purge. This modeling equation is developed in Appendix G.

Solution in MCO:

$$y = [y^0 - (n_{H_2}/n_{Ex})]e^{-\gamma t} + (n_{H_2}/n_{Ex}) \quad (P-1)$$

where: y_t = hydrogen mole fraction in the MCO void space during helium purge
 y^0 = initial hydrogen mole fraction in MCO void space
 n_{Ex} = exhaust gas rate, mole/min
 n_{H_2} = hydrogen generation rate, mole H₂/min
 P = 1 psig (15.7 psia)
 R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
 T = MCO temperature, 294 K (21°C)
 V = void space volume of the MCO, ft³
 n = total moles in MCO void space equal to PV/RT, mole
 γ = n_{Ex}/n , min⁻¹
 t = the helium purge time, min

7.8 Results

Figure 7-1 shows that it takes approximately 11 minutes, using the High Nominal hydrogen generation rate, to reach the 1% H₂ endpoint. The total flow of helium required to purge the MCO void space to a concentration at or below 0.01 mole H₂/mole gas is then easily solved by multiplying the time it takes to reach 1% H₂ with the ingress helium flow at STP. Figure 7-2 shows that it takes approximately 85 SCF, with the previous input conditions, to reach 1% H₂ in the MCO void space. Figures 7-3 shows that it takes approximately 12 minutes, using the Bounding hydrogen generation rate, to reach the 1% H₂ endpoint. Figure 7-4 shows that it takes approximately 90 SCF, with the same bounding input conditions, to reach 1% H₂ in the MCO void space.

7.9 Conclusions

Given the input parameters, the plots demonstrate that the helium purge duration will take approximately 12 minutes and 90 SCF helium to reach the 1% H₂ limit in the MCO void space, using the Bounding hydrogen gas generation rate.

7.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Figure 7-1 MCO Void Volume Transient Hydrogen Gas (H_2) Concentration During Helium Purge Prior To Vacuum Mode On Semi-Log Scale. High Nominal H_2 Generation Rate

Figure 7-2 MCO Void Volume Hydrogen Gas (H_2) Concentration During Helium Purge Measured At STP Prior To Vacuum Mode On Semi-Log Scale. High Nominal H_2 Generation Rate

Figure 7-3 MCO Void Volume Transient Hydrogen Gas (H_2) Concentration During Helium Purge Prior To Vacuum Mode On Semi-Log Scale. Bounding H_2 Generation Rate

Figure 7-4 MCO Void Volume Hydrogen Gas (H_2) Concentration During Helium Purge Measured At STP Prior To Vacuum Mode On Semi-Log Scale. Bounding H_2 Generation Rate

8.0 Evaluation of Helium Purge to Reduce Hydrogen Gas Concentrations in the MCO Void Space During Vacuum Mode

8.1 Purpose and Objectives

The purpose of this calculation is to ensure the helium purge design basis is adequate for controlling the hydrogen gas concentration at or below 4% in the MCO void space during operation.

8.2 Summary of Final Results and Conclusions

Overall mass (mole) and hydrogen balances were performed around the MCO (mass balances and mathematical derivations attached in Appendix H). An analytical solution was reached for the hydrogen mole fraction in the MCO void space (nominal 500 L) as a function of helium purge and vacuum time (Boyce and DiPrima 1969).

Based on input parameters with the minimum helium purge of 1.4 SCFM and the Bounding hydrogen generation rate, the hydrogen concentration in the MCO void space can be maintained below 4% within 5 minutes with a conservative initial hydrogen concentration of 99.8%.

8.3 Assumptions

The helium flow rate used is 1.4 SFCM; however, one case displays results of no helium purge as required. The MCO void space is evacuated at an assumed constant 30 ACFM (due to vacuum pump and/or condenser); however, the vacuum mass rate is not constant because it will vary with the MCO pressure as the total moles decrease. There is also one case where a vacuum line is assumed broken.

The hydrogen generation rates used are 1.9×10^{-3} g/sec and 2.4×10^{-3} g/sec for the high nominal and bounding values, respectively. Helium gas (assumed 100% He) is used to purge the MCO. The initial H_2 concentration is conservatively assumed to be 0.998 mole/mole total gas. Also, initial H_2 concentrations are taken at 0%. The MCO gas is assumed to be well-mixed. The initial MCO void space pressure is assumed to be 0.5 psig.

8.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626803).

8.5 Computer Model

Not applicable for this calculation.

8.6 Input Data

High Nominal (HN) H ₂ generation rate:	1.9 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
Bounding (B) H ₂ generation rate:	2.4 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
Helium ingress rate:	1.4 SCFM (Section 8.3)
Vacuum pump rate:	30 ACFM (Section 8.3)
MCO void space volume:	18 ft ³ (nominal 500 L) (Section 8.2)
MCO void space temperature:	50°C (Irwin et al 1999)
Initial MCO void space pressure:	0.5 psig (Section 8.3)

The Standard Conditions (SC) associated with the helium ingress rate is taken to be:

Temperature, T = 0°C

Pressure, P = 14.7 psia

Note that some plots display results without either helium purge or vacuum as previously noted. See Section 8.3 and EDT 626803 for input data.

8.7 Calculations

Two solutions are required for determining the hydrogen concentration in the MCO during the helium purge and vacuum and after a vacuum line break. These modeling equations are developed in Appendix H.

Solution in MCO during vacuum:

$$y = \frac{[(n_{H2}/\gamma)(e^{\gamma t} - 1) + n^0 y^0]}{[\beta(e^{\gamma t} - 1) + n^0]} \quad (P-1)$$

where: y = hydrogen mole fraction in the MCO void space during helium purge
 y^0 = initial hydrogen mole fraction in the MCO void space
 n_{He} = helium ingress rate, mole He/min
 n_{H2} = hydrogen generation rate, mole H₂/min
 V_{Ex} = actual volumetric rate of the MCO exit or exhaust gas, ft³/min
 V = void space volume of the MCO, ft³
 T = temperature of the MCO gas, K
 R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
 P = vacuum pressure down to 12 torr (0.232 psia)
 P^0 = initial pressure at 0.5 psig (15.2 psia)
 n^0 = initial total moles of gas in the MCO equal to $P^0 V / RT$, mole
 $\gamma = V_{Ex} / V$, min⁻¹
 $\beta = (n_{He} + n_{H2}) / \gamma$, mole
 t = vacuum and helium purge time, min

Solution in MCO after vacuum line break:

$$y = e^{-\gamma t} [y^0 - (n_{H2}/n_{Ex})] + (n_{H2}/n_{Ex}) \quad (B-1)$$

where: y = hydrogen mole fraction in the MCO void space after vacuum line break
 n_{Ex} = exit or exhaust gas mole rate equal to $(n_{H2} + n_{He})$, mole/min

8.8 Results

Twelve plots have been developed which display the changing H_2 concentration and MCO pressure as a function of time with the High Nominal (Figure 8-1 through 8-6) and Bounding (Figure 8-7 through 8-12) H_2 generation rates.

Figure 8-1 shows the time it would take to evacuate the MCO at the given input conditions. The minimum total pressure that can be reached in the MCO with these input parameters is approximately 1 psia. The transient H_2 partial pressure is included in this figure to compare it to the overall MCO void space pressure. Figure 8-2 shows 4% H_2 is met after 4.5 minutes with a conservative initial H_2 concentration of 99.8.

Figures 8-3 and 8-4 assume no purge helium is used. Figure 8-3 assumes the helium purge is stopped at the minimal MCO pressure of 1 psia (initial pressure for this plot) but with continued vacuum. This plot shows the minimum MCO pressure of approximately 0.027 psia is reached within five minutes. Figure 8-4 includes the same initial conditions as the previous plot. It shows the transient hydrogen concentration in the MCO void space reaches 4% (from an assumed initial 0%) in approximately 30 seconds without purge (but with continued vacuum). Figure 8-5 shows the results of continued helium purge but no vacuum (due to a broken line). This plot shows that the 4% H_2 limit can be met in approximately 50 minutes, starting with a conservative H_2 concentration of 99.8%. Figure 8-6 shows that a hydrogen concentration, in the MCO void space, over 3% cannot be reached with a broken vacuum line and continued helium purge in less than an hour, assuming the initial H_2 concentration is 0%.

Figure 8-7 shows the time it would take to evacuate the MCO at the given input conditions (Bounding H_2 rate). The minimum total pressure that can be reached in the MCO with these input parameters is approximately 1 psia. The transient H_2 partial pressure is included in this figure to compare it to the overall MCO void space pressure. Figure 8-8 shows 4% H_2 is met after 5.5 minutes with a conservative initial H_2 concentration of 99.8% and a Bounding H_2 rate.

Figures 8-9 and 8-10 assume no purge helium is used with a Bounding H_2 rate. Figure 8-9 assumes the helium purge is stopped at the minimal MCO pressure of 1 psia (initial pressure for this plot) but with continued vacuum. This plot shows the minimum MCO pressure of approximately 0.032 psia is reached within five minutes. Figure 8-10 includes the same initial conditions as the previous plot. It shows the transient hydrogen concentration in the MCO void space reaches 4% (from an assumed initial 0%) in approximately 30 seconds without purge (but with continued vacuum). Figure 8-11 shows the results of continued helium purge but no vacuum (due to a broken line). This plot shows that the 4% H_2 limit can be met in approximately 70 minutes, starting with a conservative H_2 concentration of 99.8%. Figure 8-12 shows that a hydrogen concentration, in the MCO void space, over 4% cannot be reached with a broken vacuum line and continued helium purge in over an hour (100 minutes), assuming the initial H_2 concentration is 0%.

8.9 Conclusions

Given the input parameters with the Bounding hydrogen generation rate, the plots demonstrate that a 4% hydrogen concentration in the MCO void space can be reached in less than 5.5 minutes. The minimum MCO pressure attained is approximately 1 psia (52 torr). During the vacuum mode and *no helium purge* the hydrogen concentration in the MCO void space reaches 4% in approximately 30 seconds. This assumes the H₂ concentration is initially at 0% (non-conservative bounds) when the helium is cut off; therefore, at the most, it will take only 30 seconds for the H₂ concentration to reach 4% in the MCO void space. The minimum MCO pressure attained under these conditions is approximately 0.032 psia (1.7 torr). If a break in the vacuum line should occur during the helium purge, the H₂ will reach a steady state concentration at or just below 4%. If the H₂ concentration is below 4% at the time of the break, then it cannot rise above 4% in less than 100 minutes.

8.10 References

- Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.
- Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington
- Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Figure 8-1 MCO Void Space Transient Total And H₂ Partial Pressure During Vacuum Mode And Helium Purge On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 8-2 MCO Void Space Transient Hydrogen (H₂) Concentration During Vacuum Mode And Helium Purge On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 8-3 MCO Void Space Transient Total And H₂ Partial Pressure During Vacuum Mode And No Helium Purge On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 8-4 MCO Void Space Transient Hydrogen (H₂) Concentration During Vacuum Mode And No Helium Purge On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 8-5 MCO Void Space Transient Hydrogen (H_2) Concentration During Helium Purge But No Vacuum On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 8-6 MCO Void Space Transient Hydrogen (H_2) Concentration During Helium Purge But No Vacuum On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 8-7 MCO Void Space Transient Hydrogen (H₂) Concentration During Vacuum Mode And Helium Purge On Semi-Log Scale. Bounding Hydrogen Generation Rate

Figure 8-8 MCO Void Space Transient Hydrogen (H₂) Concentration During Vacuum Mode And Helium Purge On Semi-Log Scale. Bounding Hydrogen Generation Rate

Figure 8-9 MCO Void Space Transient Total And H₂ Partial Pressure During Vacuum Mode And No Helium Purge On Semi-Log Scale. Bounding Hydrogen Generation Rate

Figure 8-10 MCO Void Space Transient Hydrogen (H₂) Concentration During Vacuum Mode And No Helium Purge On Semi-Log Scale. Bounding Hydrogen Generation Rate

Figure 8-11 MCO Void Space Transient Hydrogen (H_2) Concentration During Helium Purge But No Vacuum On Semi-Log Scale. Bounding Hydrogen Generation Rate

Figure 8-12 MCO Void Space Transient Hydrogen (H_2) Concentration During Helium Purge But No Vacuum On Semi-Log Scale. Bounding Hydrogen Generation Rate

9.0 Evaluation to Detect Leaks in MCO or Poor Vacuum Pump Performance During Vacuum Dry Mode Using Minimum Helium Purge Rate

9.1 Purpose and Objectives

The purpose of this calculation is to ensure the MCO vacuum mode design basis is adequate for which the MCO gas pressure reaches 155 torr within 5 minutes after initiating the vacuum mode at an MCO void pressure of 0.5 psig (786 torr). The hydrogen concentration must also be ensured of attaining 4% during the operation.

9.2 Summary of Final Results and Conclusions

Overall mass (mole) and hydrogen balances were performed around the MCO (mass balances and mathematical derivations attached in Appendix I). An analytical solution was reached for the hydrogen concentration in the MCO void space (nominal 500 L) as a function of helium purge and vacuum duration (Boyce and DiPrima 1969).

Based on the input parameters and Bounding hydrogen generation rate, the MCO void space pressure will adequately “pump down” to 155 torr, from an initial 0.5 psig, within 5 minutes vacuum time, as long as the vacuum rate is 15 ACFM or greater. The hydrogen concentration in the MCO void space will only reach 4% under 5 minutes with the 35 ACFM vacuum rate using the Bounding hydrogen generation rate and conservative initial hydrogen concentration of 99.8%.

9.3 Assumptions

The standard input parameters include an ingress helium rate of 1.4 SCFM and vacuum pump rates (volumetric exit gas rates at actual conditions) of 5, 10, 15, 20, 25, 30, and 35 ACFM. The hydrogen generation rates used are the High Nominal value of 1.9×10^{-3} g/sec and the Bounding value of 2.4×10^{-3} g/sec. Helium gas (assumed 100% He) is used to purge the MCO. Initial MCO pressure is 0.5 psig (786 torr) with the MCO void space pressure limit taken to be 155 torr and below. Initial H₂ concentration is conservatively taken to be 99.8%. Also, initial H₂ concentrations are taken at 0%.

9.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626803).

9.5 Computer Model

Not applicable to calculation.

9.6 Input Data

High Nominal (HN) H ₂ generation rate:	1.9 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
Bounding (B) H ₂ generation rate:	2.4 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
Helium ingress rate:	1.4 SCFM (Section 9.3)
MCO void space volume:	18 ft ³ (nominal 500 L) (Section 9.2)
MCO void space temperature:	50°C (Irwin et al 1999)
Initial MCO void space pressure:	0.5 psig (Section 9.3)

The Standard Conditions (SC) associated with the helium ingress rate is taken to be:

Temperature, T = 0°C

Pressure, P = 14.7 psia

See Section 9.3 and EDT 626803 for input data.

9.7 Calculations

Two solutions are required for determining the hydrogen concentration (mole fraction and partial pressure) in the MCO during the helium purge and vacuum. These modeling equations are developed in Appendix I.

Solution in MCO during vacuum:

$$y = \frac{[(n_{H_2}/\gamma)(e^{\gamma t} - 1) + n^0 y^0]}{[\beta(e^{\gamma t} - 1) + n^0]} \quad (P-1)$$

where: y = hydrogen mole fraction in the MCO void space during helium purge
y⁰ = initial hydrogen mole fraction in the MCO void space
n_{He} = helium ingress rate, mole He/min
n_{H₂} = hydrogen generation rate, mole H₂/min
V_{Ex} = actual volumetric rate of the MCO exit or exhaust gas, ft³/min
V = void space volume of the MCO, ft³
T = temperature of the MCO gas, K
R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
P = vacuum pressure down to 12 torr (0.232 psia)
P⁰ = initial pressure at 0.5 psig (15.2 psia)
n⁰ = initial total moles of gas in the MCO equal to P⁰V/RT, mole
γ = V_{Ex}/V, min⁻¹
β = (n_{He} + n_{H₂})/γ, mole
t = vacuum and helium purge time, min

The overall pressure change in the MCO:

$$P = (RT/V)[(P^0 V/RT) e^{-\gamma t} + \beta] \quad (PC-1)$$

with the hydrogen partial pressure in the MCO, pp_{H₂} = yP.

9.8 Results

Ten plots are presented on both linear and semi-log scale totaling twenty plots. These plots display the changing H_2 concentration (mole fraction) or partial pressure, and total MCO void space pressure as a function of vacuum time with the High Nominal (Figure 9-1a through 9-5b) and Bounding (Figure 9-6a through 9-10b) H_2 generation rates.

Figures 9-1a and 9-1b show the time to evacuate the MCO from 786 torr (0.5 psig) to 155 torr using the various volumetric vacuum pump rates with the input conditions and High Nominal H_2 generation rate. The time to reduce an initial pressure of 786 to 155 torr is less than 3 minutes using any vacuum pump rate above 15 ACFM. Figures 9-2a and 9-2b show the 99.8% initial hydrogen concentrations can be reduced to 4% H_2 in 5 minutes or less using exit flow rates of 30 ACFM or higher. To bound the initial H_2 concentration in this case, Figures 9-3a and 9-3b show that the 4% limit cannot be exceeded, as expected, if the initial H_2 concentration is below 4% (0% in this case). Figures 9-4a and 9-4b show the transient partial pressure of H_2 over the range of vacuum pump rates with the H_2 concentration beginning at 99.8%. To bound the partial pressure initial value of H_2 in this case, Figures 9-5a and 9-5b show the transient partial pressure of range of H_2 over the range of vacuum pump rates with the H_2 concentration beginning at 0%.

Figures 9-6a and 9-6b show the time to evacuate the MCO from 786 torr (0.5 psig) to 155 torr using the various volumetric vacuum pump rates with the input conditions and High Nominal H_2 generation rate. The time to reduce an initial pressure of 786 to 155 torr is less than 3 minutes using any vacuum pump rate above 15 ACFM. Figures 9-7a and 9-7b show the 99.8% initial hydrogen concentrations can be reduced to 4% H_2 in 5 minutes or less using exit flow rates of 35 ACFM or higher. To bound the initial H_2 concentration in this case, Figures 9-8a and 9-8b show that the 4% limit cannot be exceeded, as expected, if the initial H_2 concentration is below 4% (0% in this case). Figures 9-9a and 9-9b show the transient partial pressure of H_2 over the range of vacuum pump rates with the H_2 concentration beginning at 99.8%. To bound the partial pressure initial value of H_2 in this case, Figures 9-10a and 9-10b show the transient partial pressure of range of H_2 over the range of vacuum pump rates with the H_2 concentration beginning at 0%.

9.9 Conclusions

Given the input parameters with the Bounding hydrogen generation rate, the figures demonstrate that vacuum pump flow rates of 30 ACFM or higher ensures:

- 1) the pump down duration from 0.5 psig to 155 torr can be easily reached in less than 1.5 minutes,
- 2) 4% H_2 can be reached in less than 6 minutes, starting with an initial MCO void space concentration of 99.8%, and
- 3) 2 torr partial pressure of H_2 can be reached in less than 5 minutes, starting with an initial MCO void space concentration of 99.8%.

9.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Figure 9-1a MCO Void Space Transient Pressure As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. High Nominal Hydrogen Generation Rate And Initial H₂ At 99.8%

Figure 9-1b MCO Void Space Transient Pressure As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. High Nominal Hydrogen Generation Rate And Initial H₂ At 99.8%

Figure 9-2a MCO Void Space Transient Hydrogen Gas (H_2) Concentration As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. High Nominal Hydrogen Generation Rate

Figure 9-2b MCO Void Space Transient Hydrogen Gas (H_2) Concentration As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 9-3a MCO Void Space Transient Hydrogen Gas (H_2) Concentration As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. High Nominal Hydrogen Generation Rate

Figure 9-3b MCO Void Space Transient Hydrogen Gas (H_2) Concentration As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 9-4a MCO Void Space Transient Hydrogen Gas (H_2) Partial Pressure As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. High Nominal Hydrogen Generation Rate

Figure 9-4b MCO Void Space Transient Hydrogen Gas (H_2) Partial Pressure As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 9-5a MCO Void Space Transient Hydrogen Gas (H_2) Partial Pressure As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. High Nominal Hydrogen Generation Rate

Figure 9-5b MCO Void Space Transient Hydrogen Gas (H_2) Partial Pressure As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. High Nominal Hydrogen Generation Rate

Figure 9-6a MCO Void Space Transient Pressure As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. Bounding Hydrogen Generation Rate And Initial H₂ at 99.8%

Figure 9-6b MCO Void Space Transient Pressure As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. Bounding Hydrogen Generation Rate And Initial H₂ at 99.8%

Figure 9-7a MCO Void Space Transient Hydrogen Gas (H_2) Concentration As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. Bounding Hydrogen Generation Rate

Figure 9-7b MCO Void Space Transient Hydrogen Gas (H_2) Concentration As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. Bounding Hydrogen Generation Rate

Figure 9-8a MCO Void Space Transient Hydrogen Gas (H_2) Concentration As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. Bounding Hydrogen Generation Rate

Figure 9-8b MCO Void Space Transient Hydrogen Gas (H_2) Concentration As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. Bounding Hydrogen Generation Rate

Figure 9-9a MCO Void Space Transient Hydrogen Gas (H_2) Partial Pressure As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. Bounding Hydrogen Generation Rate

Figure 9-9b MCO Void Space Transient Hydrogen Gas (H_2) Partial Pressure As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. Bounding Hydrogen Generation Rate

Figure 9-10a MCO Void Space Transient Hydrogen Gas (H_2) Partial Pressure As A Function Of Exit Gas Volumetric Flow Rate On Linear Scale. Bounding Hydrogen Generation Rate

Figure 9-10b MCO Void Space Transient Hydrogen Gas (H_2) Partial Pressure As A Function Of Exit Gas Volumetric Flow Rate On Semi-Log Scale. Bounding Hydrogen Generation Rate

10.0 Evaluation of Transient Hydrogen and Air Leak Oxygen Concentrations in the MCO Void Space During Bulk Water Drain to Validate SCIC Systems Response Time

10.1 Purpose and Objectives

The purpose of this calculation is to ensure the SCIC Systems Response Time design basis is adequate for controlling the hydrogen and air leak oxygen concentrations at or below 4% in the MCO void space during the MCO bulk drain operation.

10.2 Summary of Final Results and Conclusions

Overall mass (mole), hydrogen, air (and thus, oxygen) balances were performed around the MCO void space (mass balances and mathematical derivations attached in Appendix J). Analytical solutions (Boyce and DiPrima 1969) were reached for the hydrogen and oxygen (assumed 21% of air) mole fractions in the increasing MCO void space as the bulk water drains from the MCO. The MCO contains approximately a nominal 500 L or 18 ft³ (135 gal) of water prior to drain operation.

Based on input parameters with the constant water drain at 6 gal/min (eductor data – see cut sheet in Appendix K) and the Bounding hydrogen generation rate, the hydrogen concentration in the MCO void space reaches 4% within 30 seconds, with a conservative initial hydrogen concentration of 1%, the oxygen concentration reaches 4% in approximately 10 seconds, with an initial concentration of 0%.

10.3 Assumptions

Immediately after the helium line break, the pressure within the MCO void space (0.5 to 4 psig) is assumed to reach equilibrium at 1 atm (0 psig). The helium ingress line break is conservatively assumed to break at the beginning of the bulk water drain, immediately after the helium purge.

The MCO void space increases at the same volumetric rate as the bulk water drain from the MCO. This rate is assumed constant at 6 gal/min from the eductor data. The initial hydrogen concentration is assumed to be maintained at 1% in the MCO void space at the time of the line break. The final MCO void space (at end of normal drain operation) is assumed to be 18 ft³.

10.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626115).

10.5 Computer Model

Not applicable for this calculation.

10.6 Input Data

Bounding H ₂ generation rate:	2.4 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
Initial MCO void space volume:	0.56 ft ³ (Pajunen and Klimper 1998)
MCO void space temperature:	50°C (Irwin et al 1999)
MCO void space after drain:	18 ft ³ (Section 10.3)

10.7 Calculations

Two solutions are required for determining the hydrogen and oxygen concentrations in the MCO after the helium line break. These modeling equations are developed in Appendix J.

Hydrogen mole fraction in MCO during bulk water drain:

$$y_{H_2} = \frac{[(n_{H_2} t + n^0 y^0)]}{[\alpha t + n^0]} \quad (D-1)$$

where: y_{H_2} = hydrogen mole fraction in the MCO void space during bulk water drain
 y^0 = initial hydrogen mole fraction in the MCO void space
 n_{H_2} = hydrogen generation rate, mole H₂/min
 V^0 = initial void space volume of the MCO, 0.56 ft³
 T = temperature of the MCO gas, 323 K
 R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
 P = MCO void space pressure (14.696 psia)
 n^0 = initial total moles of gas in the MCO equal to PV^0/RT , mole
 dV/dt = volumetric rate of water drain or MCO void space increase, 0.8 ft³/min
 α = $(P/RT)(dV/dt)$, moles/min
 t = vacuum and helium purge time, min

Air mole fraction in MCO void space during bulk water drain:

$$y_{air} = \frac{[(n_{air} t + n^0 y^0)]}{[\alpha t + n^0]} \quad (D-2)$$

where: y_{air} = air mole fraction in the MCO void space during bulk water drain
 y^0 = initial air mole fraction in the MCO void space

Therefore, since air is assumed to consist of 21% oxygen, the oxygen mole fraction in the MCO void space is:

$$y_{O_2} = 0.21 y_{air}$$

10.8 Results

Two plots, Figure 10-1a and 10-1b, have been developed which display the changing H₂ and O₂ concentrations as a function of drain (and line break) time with the and Bounding H₂ generation rate. Figure 10-2 shows the changing H₂ and O₂ concentrations as a function of the increasing MCO void space as the bulk water drains from the MCO.

Figure 10-1b shows it would take approximately 30 seconds to reach a flammable condition. The oxygen concentration in the MCO void space would reach the 4% limit in approximately 10 seconds and the hydrogen concentration would reach this limit in about 30 seconds after the helium line break.

Figure 10-3 shows the gas composition changes are most rapid if the helium line break were to occur at the start of the bulk water drain cycle. Several initial void volumes are used with associated transient oxygen and hydrogen concentrations.

10.9 Conclusions

Given the input parameters with the Bounding hydrogen generation rate, the plots demonstrate that a flammable condition can be reached in approximately 30 seconds after the helium line break at the beginning of the MCO bulk water drain.

Based on the assumed water removal rate, the hydrogen generation rate controls the time to achieve a flammable gas mixture for the line break scenario.

10.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems*, Second Edition, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Pajunen, A. L. and Klimper, S. C., 1998, *Inert Gas Requirements For Cask Loading*, HNF-2833, Rev. 0, COGEMA Engineering Corporation, Richland, Washington.

Figure 10-1a MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Helium Line Break (Air Ingress) During MCO Bulk Water Drain. Bounding H_2 Generation Rate

Figure 10-1b MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Helium Line Break (Air Ingress) During MCO Bulk Water Drain. Bounding H_2 Generation Rate

Figure 10-2 MCO Void Space Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Increasing MCO Void Space Due To Bulk Water Drain . Bounding H_2 Generation Rate

Figure 10-3 MCO Void Space Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Increasing MCO Void Space Due To Bulk Water Drain . Bounding H_2 Generation Rate

11.0 Evaluation of Transient MCO Void Space Hydrogen and Air Leak Oxygen Concentrations After Bulk Water Drain to Validate SCIC Systems Response Time

11.1 Purpose and Objectives

The purpose of this calculation is to ensure the SCIC Systems Response Time design basis is adequate for controlling the hydrogen gas and air leak oxygen concentrations at or below 4% in the MCO void space after the MCO bulk water drain.

11.2 Summary of Final Results and Conclusions

Overall mass (mole), hydrogen, and air balances were performed around the MCO void space (mass balances and mathematical derivations attached in Appendix K). Four first order differential equations were developed to model transient gas compositions during a hypothetical air leak event. A numerical method was used to determine the hydrogen concentration in the MCO void space since an analytical solution was not apparent. The numerical solution utilizes a Runge-Kutta (RK) method for finding an approximate solution to the first order differential equations.

Based on input parameters, including a Bounding hydrogen generation rate, the oxygen and hydrogen gas concentrations in the MCO void space reach 4% each, approximately 3.5 minutes after a helium line break with an air leak ingress rate of 0.35 SCFM. Lesser air leak rates shorten the time for hydrogen but increase the time for oxygen to reach 4%. Hydrogen reaches 4%, with no or very little air leakage, in approximately 3 minutes after the helium line is broke open to ambient air. Higher air leak rates decrease the time for oxygen to reach 4% but increase the time for the hydrogen to reach 4% to a point when the air leak rate is 1.4 SCFM. At this rate and above, the hydrogen concentration cannot reach 4% since it is diluted with ingress air; therefore, a pipe break causing air ingress at 0.35 SCFM into the drained MCO configuration results in the shortest time to produce a flammable gas mixture.

11.3 Assumptions

Assuming the MCO is drained of bulk water with continued eductor operation while the helium line is damaged and opened to ambient air, the initial void space pressure is assumed to be at 1 atm (14.7 psia) with the initial hydrogen and oxygen concentrations at 1% and 0%, respectively. The constant Bounding hydrogen generation rate of 2.4×10^{-3} g/sec is used at an MCO temperature of 50°C (122°F). The MCO void space is assumed to be a nominal 500 L (18 ft³). A flammable gas mixture is assumed to be observed when the concentration of both hydrogen and oxygen exceed 4%.

The eductor (or Water Jet Exhauster), which controls the exhaust flow out of the MCO, is assumed to operate with motive water at 60 psig and 80°F. The eductor operation curve (suction pressure vs. air capacity) data was taken from the cut sheet information (see Appendix K) and described as a quadratic by a 2nd order least squares fit (see Figure 11-6). The MCO void space pressure as a function of the exhaust rate is therefore described as:

$$P \text{ (in Hg)} = a_0 + a_1 V + a_2 V^2 \quad (\text{Q-1})$$

where: $a_0 = 1.7858 \text{ in Hg}$

$$a_1 = 2.9729 \frac{\text{in Hg min}}{\text{ft}^3}$$

$$a_2 = -0.0706 \frac{\text{in Hg min}^2}{\text{ft}^6}$$

converting volumetric flow units (at SCFM) to mole units ($n = PV/RT$) and pressure (in Hg) to (psia):

$$P(\text{psia}) = a'_0 + a'_1 n_{\text{ex}} + a'_2 n_{\text{ex}}^2 \quad (\text{Q-2})$$

where: $a'_0 = 0.8772 \text{ psia}$

$$a'_1 = 1.1554 \frac{\text{psia min}}{\text{mole}}$$

$$a'_2 = -0.0217 \frac{\text{psia min}^2}{\text{mole}^2}$$

11.4 Software Applications

MATLAB was used to solve and plot the RK numerical method results (see files in EDT 626115). The same RK method was used previously in Section 1.0 of this document and proven consistent with analytical results (see Section 1.4, Software Applications).

11.5 Computer Model

See Section 11.4 for modeling application and EDT 626115 for MATLAB plotting routines and Runge-Kutta subroutines.

11.6 Input Data

Bounding H ₂ generation rate:	2.4 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
MCO void space volume:	18 ft ³ (Section 11.3)
MCO void space temperature:	50°C (Irwin et al 1999)

11.7 Calculations

Four first order differential equations are required for determining the hydrogen and oxygen concentrations in the MCO after the helium line break. These modeling equations are developed in Appendix K. The four equations solved by the RK numerical are:

$$\frac{dn_{ex}}{dt} = \frac{(\alpha - n_{ex})(RT/V)}{(a'_1 + 2 a'_2 n_{ex})} \quad (D-1)$$

$$\frac{dn}{dt} = \alpha - n_{ex} \quad (D-2)$$

$$\frac{dy_{air}}{dt} = (1/n)(n_{air} - n_{ex}y_{air} - y_{air} \frac{dn}{dt}) \quad (D-3)$$

$$\frac{dy_{H_2}}{dt} = (1/n)(n_{H_2} - n_{ex}y_{H_2} - y_{H_2} \frac{dn}{dt}) \quad (D-4)$$

The oxygen fraction, $[O_2]$, in the MCO void space is therefore equal to:

$$y_{O_2} = 0.21y_{air}$$

where:

n_{ex} = mole exhaust rate from the MCO void space, mole/min
 n_{ex}^0 = initial mole exhaust rate from the MCO void space, mole/min
 n = total moles of gas in the MCO void space, mole
 n^0 = initial total moles of gas in the MCO void space (P^0V/RT), mole
 y_{air} = mole fraction of air in MCO void space, mole air/total moles
 y_{air}^0 = mole fraction of air in MCO void space, mole air/total moles
 y_{H_2} = mole fraction of hydrogen in MCO void space, mole H_2 /total moles
 $y_{H_2}^0$ = initial mole fraction of hydrogen in MCO void space, 0.01 mole H_2 /total moles
 y_{O_2} = mole fraction of oxygen in MCO void space, mole O_2 /total moles
 $y_{O_2}^0$ = initial mole fraction of oxygen in MCO void space, 0 mole O_2 /total moles
 n_{air} = ingress moles of air during air leak, mole air/min
 n_{H_2} = hydrogen generation rate, mole H_2 /min
 α = $n_{air} + n_{H_2}$, moles of hydrogen and air/min
 P^0 = initial MCO pressure right after helium line break, 14.7 psia
 V = MCO void space, 18 ft³
 T = temperature of the MCO gas, 323 K
 R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
 t = time during eductor operation and air leak, min

The initial exhaust rate (n_{ex}^0) is determined by solving the roots to the quadratic (equation Q-2 with $P = P^0$) and using one of the logical roots in the eductor operation. Figure 11-7 shows the initial exhaust mole rate to be 18.14 mole/min. This is the logical choice since the pressure and mole/min must both decrease as the eductor operates. The second root of 35.10 mole/min could not be possible as an initial exhaust mole rate since the pressure in the MCO shows an increase as the exhaust rate of moles of gas in the MCO decrease.

11.8 Results

Figures 11-2 through 11-5 show the transient hydrogen and oxygen concentration after the helium line breaks and ingress air begins to invade the MCO void space. For a bounding hydrogen increase comparison, Figure 11-1 shows the hydrogen increase without an air ingress leak. For smaller leaks, as shown in Figure 11-2, the oxygen concentration controls the time to reach a flammable condition. The “worst case” condition or quickest time for both oxygen and hydrogen to reach 4% is at approximately 3.5 minutes after the helium line break, when the air ingress rate is at 0.35 SCFM with input conditions. This condition is shown in Figure 11-3. Figure 11-4 shows as the leak rate is increased to 1.2 SCFM, the oxygen concentration, as expected, quickly increases but the hydrogen concentration becomes diluted and decreases at a level just above 4%. When the leak rate is 1.4 SCFM, as shown in Figure 11-5, the hydrogen concentration is further diluted and falls below 4%. Any air leak rate 1.4 SCFM and higher will dilute the generated hydrogen and limit it to below 4%. The air leak rate is limited by either the eductor or by the pipe break. If the eductor limits, then the flow rate, n_{ex} , is much greater than the 0.35 SCFM air leak rate.

11.9 Conclusions

Given the input parameters with the Bounding hydrogen generation rate, the plots demonstrate that a flammable condition can be reached in a “worst case” air leak (0.35 SCFM) approximately 3.5 minutes after the helium line break. This scenario assumes the break occurs right after the bulk water is drained from the MCO with the eductor still in operation.

11.10 References

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Figure 11-1 MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Helium Line Break (Air Ingress) After MCO Bulk Water Drain. Bounding H_2 Generation Rate

Figure 11-2 MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Helium Line Break (Air Ingress) During MCO Bulk Water Drain. Bounding H_2 Generation Rate

Figure 11-3 MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Helium Line Break (Air Ingress) During MCO Bulk Water Drain. Bounding H_2 Generation Rate

Figure 11-4 MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Helium Line Break (Air Ingress) During MCO Bulk Water Drain. Bounding H_2 Generation Rate

Figure 11-5 MCO Void Space Transient Hydrogen Gas (H₂) And Oxygen (O₂) Concentrations As A Function Of Helium Line Break (Air Ingress) During MCO Bulk Water Drain. Bounding H₂ Generation Rate

Figure 11-6 Least Squares Fit Using 2" Diameter Eductor Data With Motive Water at 60 Psig and 80°F

Figure 11-7 MCO Pressure As A Function Of Mole Exhaust Rate As Determined By The Eductor.
The Initial Mole Exhaust Rate At The Initial Pressure Is Determined To Be 18.14 Mol/Min

12.0 "Ideal" Mixing of Minimum Helium Purge to Reduce Hydrogen and Oxygen Concentrations in the MCO Void Space After a Vacuum Line Break

12.1 Purpose and Objectives

The purpose of this calculation is to ensure the helium purge design basis is adequate for controlling the hydrogen and oxygen concentration at or below 4% in the MCO void space after a vacuum line break. This evaluation assumes "ideal" mixing and Section 20 assumes "non-ideal" mixing of hydrogen gas with helium purge and leak oxygen.

12.2 Summary of Final Results and Conclusions

Overall mass (mole), air (thus, oxygen), and hydrogen balances were performed around the MCO void space (mass balances and mathematical derivations attached in Appendix L). Analytical solutions (Boyce and DiPrima 1969) were developed for the air leak oxygen (caused by a vacuum line break) and hydrogen mole fractions in the MCO void space (nominal 500 L) as a function of helium purge and air leak time.

Based on input parameters with the minimum helium purge of 1.4 SCFM and the Bounding hydrogen generation rate, the hydrogen concentration in the MCO void space can always be maintained below 4% with the oxygen reaching below 4% after approximately 25 minutes. A lesser helium flow, such as 1.0 SCFM, results in the hydrogen rising above 4% after 28 minutes and the oxygen falling below 4% after 33 minutes.

12.3 Assumptions

The vacuum line is assumed broken during vacuum process, whereby, an initial condition assumes the MCO void space immediately fills with air at 1 atm. The broken vacuum line is assumed to be quickly shut off, with the MCO filled with air at 1 atm, and the helium purge begins with the safety class exhaust valve set at 4 psig. A Bounding hydrogen generation rate is used. Helium gas (assumed 100% He) is used to purge the MCO. The initial H₂ concentration is assumed to be 0. The MCO gas is assumed to be well-mixed.

12.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626115).

12.5 Computer Model

Not applicable for this calculation.

12.6 Input Data

Bounding H ₂ generation rate:	2.4 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
MCO void space volume:	18 ft ³ (nominal 500 L) (Section 12.2)
MCO void space temperature:	50°C (Irwin et al 1999)
Initial MCO void space pressure:	14.7 psia (1 atm)(Section 12.3)
Final (Steady State) MCO void space pressure:	18.7 psia (4 psig)(Section 12.3)

The Standard Conditions (SC) associated with the helium ingress rate is taken to be:

Temperature, T = 0°C

Pressure, P = 14.7 psia

12.7 Calculations

Four solutions are required for determining the hydrogen and oxygen concentration in the MCO during the helium purge and air leak ingress after a vacuum line break. Two solutions are required for the pressure rise duration and two solutions are required for the constant pressure (steady state) duration. These modeling equations are developed in Appendix L.

Air mole fraction in MCO void space during pressure rise from 0 psig to 4 psig:

$$y_{\text{air}} = \frac{n^0 y^0}{[\alpha t + n^0]} \quad (\text{P-1})$$

where: y_{air} = air mole fraction in the MCO void space during pressure rise
 y^0 = initial air mole fraction in the MCO void space
 V = void space volume of the MCO, 18 ft³
 P^0 = initial MCO void space pressure, 14.7 psia
 T = temperature of the MCO gas, 323 K
 R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
 n_{He} = helium ingress rate, mole He/min
 n_{H_2} = hydrogen generation rate, mole H₂/min
 n^0 = initial moles of gas in the MCO void space, $P^0 V / RT$, mole
 α = $(n_{\text{He}} + n_{\text{H}_2})$, mole/min
 dV/dt = volumetric rate of water drain or MCO void space increase, 0.8 ft³/min (6 gal/min)
 α = $(P/RT)(dV/dt)$, moles/min
 t = helium purge time after vacuum line break, min

Therefore, the oxygen mole fraction, assumed 21% of air, in the MCO void space is:

$$y_{\text{O}_2} = 0.21 y_{\text{air}}$$

Hydrogen mole fraction in MCO void space during pressure rise from 0 psig to 4 psig:

$$y_{\text{H}_2} = \frac{[(n_{\text{H}_2} t + n^0 y^0)]}{[\alpha t + n^0]} \quad (\text{P-2})$$

where: y_{H_2} = hydrogen mole fraction in the MCO void space during pressure rise
 y^0 = initial hydrogen mole fraction in the MCO void space

Air mole fraction in MCO void space at constant pressure:

$$y_{\text{air}} = y_{\text{air}}^0 e^{-\phi t} \quad (\text{S-1})$$

where: y_{air} = air mole fraction in the MCO void space
 y_{air}^0 = initial air mole fraction in the MCO void space
 P = steady state MCO void space pressure, 18.7 psia
 n = total moles of gas in MCO void space, PV/RT , mole
 $\phi = \alpha/n$, min^{-1}
 t = helium purge time, min

Therefore, the oxygen mole fraction, assumed 21% of air, in the MCO void space is:

$$y_{\text{O}_2} = 0.21 y_{\text{air}}$$

Hydrogen mole fraction in MCO void space at constant pressure:

$$y_{\text{H}_2} = [y_{\text{H}_2}^0 - (n_{\text{H}_2}/\alpha)] e^{-\phi t} + (n_{\text{H}_2}/\alpha) \quad (\text{S-2})$$

where: y_{H_2} = hydrogen mole fraction in the MCO void space
 $y_{\text{H}_2}^0$ = initial hydrogen mole fraction in the MCO void space

12.8 Results

A parametric analysis using various helium purge flow is presented in four figures. Figure 12-1 uses a helium ingress flow of 0.5 SCFM. The hydrogen concentration reaches 4% in approximately 16 minutes with the given input conditions. The oxygen concentration is still well above 4% (~13%) at this time. When the helium ingress rate is 1.0 SCFM, Figure 12-2 shows the hydrogen concentration reaches 4% in approximately 25 minutes while the oxygen concentration falls below 4% in approximately 30 minutes. In the final two figures, with the helium rate at 1.4 and 3.0 SCFM, the hydrogen concentration does not go beyond 4% while the oxygen concentration falls to 4% in 22 and 10 minutes, respectively.

12.9 Conclusions

Given the input parameters with the Bounding hydrogen generation rate, the plots demonstrate, assuming "ideal" mixing, that the hydrogen concentration in the MCO void space, after an air ingress leak, can be maintained indefinitely below 4% with a minimum helium purge rate of 1.4 SCFM.

12.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Figure 12-1 MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Minimum Helium Purge After Vacuum Line Break. Bounding H_2 Gen. Rate

Figure 12-2 MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Minimum Helium Purge After Vacuum Line Break. Bounding H_2 Gen. Rate

Figure 12-3 MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Minimum Helium Purge After Vacuum Line Break. Bounding H_2 Gen. Rate

Figure 12-4 MCO Void Space Transient Hydrogen Gas (H_2) And Oxygen (O_2) Concentrations As A Function Of Minimum Helium Purge After Vacuum Line Break. Bounding H_2 Gen. Rate

13.0 Evaluation of Cask Vent Line Orifice Diameter

13.1 Purpose and Objectives

The purpose of this calculation is to determine the orifice diameter size in the Cask vent line based on the allowable hydrogen concentration in the HVAC duct receiving the vent exhaust gas.

13.2 Summary of Final Results and Conclusions

The Cask vent line orifice size limiting the mass flow of gas entering the HVAC system varies with the assumed maximum receipt pressure. Table 13-1 summarizes alternative orifice sizes supporting selected constraints.

Table 13-1

Cask Vent Flow (SCFM)	Assumed Maximum Receipt Pressure (psig)	Orifice Diameter (inches)
10	150	0.041
10	20	0.088
40	150	0.081
40	20	0.176

13.3 Assumptions

It is assumed the nominal HVAC flow rate is 1000 SCFM. To remain at 1% or 4% hydrogen in the HVAC System the vent flow determined is 10 and 40 SCFM, respectively. The 150 psig of gas vented from the MCO/Cask is assumed to consist of 100% hydrogen. The orifice is assumed to be frictionless releasing a constant gas reservoir of 150 psig. Hydrogen gas in MCO/Cask assumed ideal.

13.4 Software Applications

MATLAB software was utilized to plot the data generated from the calculated solutions (see EDT 626115).

13.5 Computer Model

Not applicable for this calculation.

13.6 Input Data

MCO void space volume:	0.56 ft ³ (Pajunen and Klimper 1998)
Cask void space volume:	0.53 ft ³ (Pajunen and Klimper 1998)
MCO/Cask void space temperature:	50°C (Irwin et al 1999)

13.7 Calculations

The orifice diameter determined at 150 psig Cask pressure and 10 SCFM (or 40 SCFM) vent as:

$$D = \sqrt{(4/\pi)(m/G_{NZ})} \quad (\text{Levenspiel 1984}) \quad (\text{D-1})$$

where: D = diameter of Cask vent orifice, in
 m = mass flow rate through the orifice at 10 or 40 SCFM, lb_m/min
 G_{NZ} = mass flow rate per orifice area, lb_m/min in²

The following equation is the mass flow rate for 10 and 40 SCFM used above accordingly:

$$m = \frac{PV(MW)}{RT} \quad (\text{M-1})$$

where: P = 1 atm (at standard conditions)
 V = 10 or 40 SCFM (ft³/min at standard conditions)
 MW = molecular weight of hydrogen gas, 2 lb_m/lbmol
 R = ideal gas constant, 0.729 ft³ atm/ lbmol °R
 T = 491 °R (273 K) standard temperature

The above equations (D-1) and (M-1) are also used for the MCO/Cask pressure of 20 psig during the purge/vent cycles in place of the initial 150 psig upon CVDF receipt.

Input calculations can be found in Appendix M.

13.8 Results

Two different MCO/Cask venting scenarios are used in the orifice size determination. The first is the most conservative case where the MCO/Cask is vented upon receipt and the maximum design pressure of 150 psig is used. The second case is where the MCO/Cask is at the first purge/vent cycle from 0.5 psig to 20.5 psig as previously shown in Section 1 of this document. However, note that the problem in Section 1 did not use any venting restrictions in regard to exceeding HVAC hydrogen gas concentrations (i.e., 10 SCFM or 40 SCFM).

Figures 13-1 and 13-2 determine Cask vent orifice sizes conservatively using 150 psig in the MCO/Cask void space at vent flow limits of 10 and 40 SCFM, respectively. The orifice diameter size for the limit of 10 SCFM is 0.041" and for the limit of 40 SCFM is 0.081".

Figures 13-3 and 13-4 determine Cask vent orifice sizes conservatively using 20 psig in the MCO/Cask void space at vent flow limits of 10 and 40 SCFM, respectively. The orifice diameter size for the limit of 10 SCFM is 0.088" and for the limit of 40 SCFM is 0.176".

13.9 Conclusions

The Cask vent orifice has been determined for two different MCO/Cask pressure scenarios, 150 psig and 20 psig. An orifice designed for 150 psig is not an operationally realistic size for a considerably lower pressure such as 20 psig. The purge/vent process used in Section 1 of this document does not take into consideration the orifice size for the vent operation. Section 1 assumes the helium purge duration is equal to the vent duration. An orifice sized for 150 psig reservoir pressure will take considerably longer to vent if used with a 20 psig reservoir.

13.10 References

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Levenspiel, O., 1984, *Engineering Flow and Heat Exchange*, Plenum Press, New York, New York.

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Pajunen, A. L. and Klimper, S. C., 1998, *Inert Gas Requirements For Cask Loading*, HNF-2833, Rev. 0, COGEMA Engineering Corporation, Richland, Washington.

Figure 13-1 Cask Vent Orifice Diameter As A Function Of Maximum Cask/MCO Void Space Pressure And Flow Limit Of 10 SCFM

Figure 13-2 Cask Vent Orifice Diameter As A Function Of Maximum Cask/MCO Void Space Pressure And Flow Limit Of 40 SCFM

Figure 13-3 Cask Vent Orifice Diameter As A Function Of 20 Psig Cask/MCO Void Space Pressure And Flow Limit Of 10 SCFM

Figure 13-4 Cask Vent Orifice Diameter As A Function Of 20 Psig Cask/MCO Void Space Pressure And Flow Limit Of 40 SCFM

14.0 Evaluation of Transient Hydrogen Concentration in the MCO Void Space Before Bulk Water Drain During MCO Isolation Delay

14.1 Purpose and Objectives

The purpose of this calculation is to determine how long the helium purge can be shut off during the drying operation without generating a gas mixture that would be potentially flammable in the event of an air ingress.

14.2 Summary of Final Results and Conclusions

Overall mass (mole) and hydrogen balances were performed around the MCO void space (mass balances and mathematical derivations attached in Appendix N). Analytical solutions (Boyce and DiPrima 1969) were reached for the hydrogen mole fractions in the MCO void space as the vacuum operation continues after the helium purge is shut down.

If the helium ingress purge is shut off after having reached steady state with a minimum helium purge at 1.4 SCFM and vacuum flow rates at or above 5 ACFM, the partial pressure of hydrogen will remain below 12 torr (see Section 19 regarding the 12 torr limit). Calculations show the partial pressure of hydrogen remains constant at a constant vacuum rate with no helium purge (see Appendix N).

14.3 Assumptions

The helium is assumed shut off when the partial pressure of hydrogen reaches steady state at a specified vacuum rate. The helium flow purge is assumed to be 1.4 SCFM prior to being shut off. The Bounding hydrogen generation rate is used. The MCO contains a nominal 500L or 18 ft³ of void space.

14.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626115).

14.5 Computer Model

Not applicable for this calculation.

14.6 Input Data

Bounding H ₂ generation rate:	2.4 x 10 ⁻³ g H ₂ /sec (Pajunen 1998)
MCO void space:	18 ft ³ (Section 14.3)
MCO void space temperature:	50°C (Irwin et al 1999)

14.7 Calculations

Three different vacuum flow rates are compared. For each vacuum flow rate, a hydrogen concentration needs to be determined at steady state to be used as the initial hydrogen fraction in the modeling equation. These modeling equations are developed in Appendix N.

The hydrogen mole fraction in the MCO void space during the vacuum operation with no helium purge is as follows:

$$y_{H_2} = \frac{[(n_{H_2}/k)(e^{kt} - 1) + n^0 y^0]}{[(n_{H_2}/k)(e^{kt} - 1) + n^0]} \quad (V-1)$$

where: y_{H_2} = hydrogen mole fraction in the MCO void space during vacuum with no helium purge
 y^0 = initial hydrogen mole fraction in the MCO void space at start of no helium purge, $n_{H_2}/(n_{H_2} + n_{He})$
 n_{He} = helium purge rate, mole He/min
 n_{H_2} = hydrogen generation rate, mole H_2 /min
 V = MCO void space volume, 18 ft³
 V_{ex} = vacuum flow rate, ft³/min (actual conditions)
 T = MCO gas temperature, 323 K
 R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
 P^0 = initial MCO void space pressure at start of helium shut off, $(n_{H_2} + n_{He})RT/V_{ex}$
 n^0 = initial total moles of gas in the MCO equal to P^0V/RT , mole
 $k = V_{ex}/V$, min⁻¹
 t = vacuum time, min

14.8 Results

Figures 14-1 and 14-2 show these initial hydrogen partial pressures and mole fractions, respectively, as steady state is attained for each vacuum rate *with* helium purge and initial input parameters. After the helium purge is shut off the partial pressure of hydrogen remains constant while the hydrogen mole fraction quickly reaches 1.0 (100% H_2). Figure 14-3 displays the hydrogen mole fraction at various vacuum flow rates with the helium purge shut off. The initial hydrogen fraction used for each vacuum rate in this figure was taken at the steady state condition of 4% shown in Figure 14-2.

14.9 Conclusions

Given the input parameters with the Bounding hydrogen generation rate, the plots demonstrate that the hydrogen partial pressure can be maintained below 12 torr with any vacuum rate at 5 ACFM or above.

14.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Pajunen, A. L. and Klimper, S. C., 1998, *Inert Gas Requirements For Cask Loading*, HNF-2833, Rev. 0, COGEMA Engineering Corporation, Richland, Washington.

**Figure 14-1 MCO Void Space Hydrogen Partial Pressure Per Vacuum Rate Attaining Steady State.
Bounding Hydrogen Generation Rate**

**Figure 14-2 MCO Void Space Hydrogen Concentration Per Vacuum Rate Attaining Steady State.
Bounding Hydrogen Generation Rate**

Figure 14-3 MCO Void Space Transient Hydrogen Concentration During Vacuum Operation With Helium Purge Shut Off. Bounding Hydrogen Generation Rate

15.0 Evaluation of Transient Hydrogen Concentrations in the MCO Void Space During MCO Isolation Period Before Bulk Water Drain

15.1 Purpose and Objectives

The purpose of this calculation is to ensure the design is adequate for maintaining the hydrogen concentrations at or below 4% in the MCO void space during the MCO isolation period prior to the bulk drain operation.

15.2 Summary of Final Results and Conclusions

Overall mass (mole) and hydrogen balances were performed around the MCO void space (mass balances and mathematical derivations attached in Appendix O). An analytical solution (Boyce and DiPrima 1969) was reached for the hydrogen mole fraction in the MCO void space during the isolation period.

The hydrogen concentration in the MCO void space increases from 1% to 4% in approximately 16 seconds during the MCO isolation period using the Bounding hydrogen generation rate.

15.3 Assumptions

The Bounding hydrogen generation rate of 2.4×10^{-3} g H₂/sec (Pajunen 1998) is used. The initial hydrogen concentration is assumed to be 1% in the MCO void space. The MCO void space is assumed to have an initial pressure of 0.5 psig prior to the isolation period.

15.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626115).

15.5 Computer Model

Not applicable for this calculation.

15.6 Input Data

Bounding H ₂ generation rate:	2.4×10^{-3} g H ₂ /sec (Pajunen 1998)
MCO void space volume:	0.56 ft ³ (Pajunen and Klimper 1998)
MCO void space temperature:	50°C (Irwin et al 1999)

15.7 Calculations

One solution was required for determining the hydrogen concentration in the MCO void space during the isolation period. This modeling equation is developed in Appendix O. Hydrogen mole fraction in MCO during isolation period:

$$y_{H_2} = \frac{[(n_{H_2} t + n^0 y^0)]}{[n_{H_2} t + n^0]} \quad (I-1)$$

where: y_{H_2} = hydrogen mole fraction in the MCO void space during isolation period
 y^0 = initial hydrogen mole fraction in the MCO void space
 n_{H_2} = hydrogen generation rate, mole H_2 /min
 V = MCO void space volume, 0.56 ft³
 T = MCO gas temperature, 323 K
 R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
 p^0 = initial MCO void space pressure, 15.2 psia (0.5 psig)
 n^0 = initial total moles of gas in the MCO equal to $P^0 V / RT$, mole
 t = isolation time, min

15.8 Results

Figure 15-1 displays the changing H_2 concentration in the MCO void space as a function of the isolation period. The initial hydrogen concentration at 1% takes approximately 16 seconds to reach the 4% concentration limit using the Bounding hydrogen generation rate. Figure 15-2 shows the transient hydrogen concentration over 30 minutes of isolation time. Figure 15-3 shows the pressure increase in the MCO void space over 30 minutes.

15.9 Conclusions

Given the input parameters with the Bounding hydrogen generation rate, the plots demonstrate that a 4% hydrogen concentration in the MCO void space can be reached in approximately 16 seconds if the MCO is isolated during the bulk water drain process step.

15.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Pajunen, A. L. and Klimper, S. C., 1998, *Inert Gas Requirements For Cask Loading*, HNF-2833, Rev. 0, COGEMA Engineering Corporation, Richland, Washington.

Figure 15-1 MCO Void Space Transient Hydrogen Concentration During MCO Isolation Period Prior To Bulk Water Drain. Bounding Hydrogen Generation Rate

Figure 15-2 MCO Void Space Transient Hydrogen Concentration During MCO Isolation Period Prior To Bulk Water Drain. Bounding Hydrogen Generation Rate

Figure 15-3 MCO Void Space Pressure Over MCO Isolation Period Prior To Bulk Water Drain.
Bounding Hydrogen Generation Rate

16.0 Evaluation of Transient Hydrogen Concentrations in the HVAC Duct During MCO/Cask Vent Operation

16.1 Purpose and Objectives

The purpose of this calculation is to determine how long the HVAC system can be shut down (power off) during MCO/Cask vent operations.

16.2 Summary of Final Results and Conclusions

Overall mass (mole) and hydrogen balances were performed around an HVAC volume (mass balances and mathematical derivations attached in Appendix P) receiving the MCO/Cask vent gas. An analytical solution (Boyce and DiPrima 1969) was reached for the hydrogen mole fraction in the specified HVAC duct volume.

The hydrogen concentration in the HVAC duct section takes approximately 1.2 seconds to reach the 4% concentration limit with the vent flow restricted to 10 SCFM and the hydrogen concentration takes approximately 0.28 seconds to reach the 4% concentration limit with the vent flow restricted to 40 SCFM.

16.3 Assumptions

The MCO/Cask vent gas is analyzed in the first ten feet of cylindrical duct (volume of 10 linear feet 10 inches in diameter referred to as the "duct section"). This is the approximate duct dimension from the MCO/Cask to the main leg of HVAC duct in the CVDF. The duct section is analyzed as a steady state "open end" volume. The maximum vent rate assumed is 40 SCFM with 10 SCFM also utilized. These vent flows are restricted by the Cask vent orifice sizes determined in Section 13.

The conservative initial hydrogen concentration is assumed to be 100% in the MCO/Cask void space and 0% in the HVAC duct. This assumption pertains to the first vent operation or cycle per MCO/Cask when the HVAC duct contains the lowest concentration of hydrogen and the MCO/Cask void space contains the highest concentration of hydrogen. The gas temperature in the HVAC duct section is assumed to be 50°C.

Two MCO/Cask vent scenarios are analyzed. In the first case, the MCO/Cask void space is assumed to have a maximum pressure of 150 psig upon initial vent to the HVAC. In the second case, the MCO/Cask void space is assumed to have a maximum pressure of 20 psig during the MCO/Cask purge/vent operation at the initial purge/vent cycle (see Section 1.0).

16.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626115).

16.5 Computer Model

Not applicable for this calculation.

16.6 Input Data

HVAC duct section volume:	5.45 ft ³ (Section 16.3 and see below calc)
HVAC duct section gas temperature:	50°C (Section 16.3)
Vent volumetric rate (100% H ₂)	10 and 40 SCFM (Section 16.3)
No initial hydrogen in duct	(Section 16.3)

HVAC duct section used in mass balance:

$$V_{\text{HVAC}} = (\pi/4) D^2 \times L = (\pi/4) [10 \text{ in.}(1 \text{ ft}/12 \text{ in.})]^2 \times 10 \text{ ft} = 5.45 \text{ ft}^3$$

16.7 Calculations

One solution was required for determining the hydrogen concentration in the duct section receiving the MCO/Cask vent gas. This modeling equation is developed in Appendix P.

Hydrogen mole fraction in MCO during isolation period:

$$y_{\text{H}_2} = (y^0 - 1)e^{-kt} + 1 \quad (\text{I-1})$$

where: y_{H_2} = hydrogen mole fraction in the HVAC duct section during vent operation
 y^0 = initial hydrogen mole fraction in the HVAC duct section
 n_{H_2} = hydrogen vent rate, mole H₂/min
 n = total moles of gas in the HVAC duct section, PV/RT, mole
 P = HVAC duct section pressure (14.696 psia)
 V = HVAC duct section volume, 5.45 ft³
 T = temperature of the HVAC duct section gas, 323 K
 R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)
 $k = n_{\text{H}_2}/n$, min⁻¹
 t = vent time, min

16.8 Results

Figures 16-1 and 16-2 display the transient H₂ concentration, assuming constant pressure, in the duct section with vent rates of 10 and 40 SCFM, respectively. In Figure 16-1, the hydrogen concentration takes approximately 1.2 seconds to reach the 4% concentration limit with the given input conditions. In Figure 16-2, the hydrogen concentration takes approximately 0.28 seconds to reach the 4% concentration limit with the given input conditions.

Figures 16-3 and 16-4 display the transient H₂ concentration in the assumed steady state gas volume (constant pressure) over 30 seconds of vent operation in the duct section with vent rates of 10 and 40 SCFM, respectively.

16.9 Conclusions

Given the input parameters with the two venting rates, the plots demonstrate that a 4% hydrogen concentration in the duct section can be reached as early as 0.28 seconds, determined by the gas release rate.

16.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Figure 16-1 10' HVAC Duct Section Transient Hydrogen Concentration During 10 SCFM Vent From MCO/Cask Void Space. HVAC Volume Assumed Open To Steady State Flow

Figure 16-2 10' HVAC Duct Section Transient Hydrogen Concentration During 40 SCFM Vent From MCO/Cask Void Space. HVAC Volume Assumed Open To Steady State Flow

Figure 16-3 10' HVAC Duct Section Transient Hydrogen Concentration During 10 SCFM Vent From MCO/Cask Void Space Over 30 Seconds

Figure 16-4 10' HVAC Duct Section Transient Hydrogen Concentration During 40 SCFM Vent From MCO/Cask Void Space Over 30 Seconds

17.0 Evaluation of MCO Pressure Rise and Transient Hydrogen Concentration Following Vacuum Operation Using Minimum Helium Purge

17.1 Purpose and Objectives

The purpose of this calculation is to ensure the design basis demonstrates an adequate pressure rise during minimal helium purge in the MCO after the vacuum operation. The transient hydrogen concentration is also evaluated to ensure it remains at or below 4% during the helium purge.

17.2 Summary of Final Results and Conclusions

Overall mass (mole) and hydrogen balances were performed around the MCO (mass balances and mathematical derivations attached in Appendix Q). An analytical solution (Boyce and DiPrima 1969) was reached for the hydrogen mole fraction in the MCO during the helium purge.

It takes approximately 11 minutes to fill the MCO, with the helium purge at 1.4 SCFM, beginning at 12 torr and ending at 786 torr (0.5 psig). With the helium purge at 3 SCFM, it takes approximately 5 minutes to meet these same pressure limits.

A minimal helium purge rate at 1.4 SCFM is required to keep the hydrogen concentration below 4%. A helium purge rate of 6 SCFM or higher is required to maintain the MCO hydrogen concentration at 1% or lower.

17.3 Assumptions

The constant Bounding hydrogen generation rate of 2.4×10^{-3} g/sec is used at an MCO temperature of 50°C (122°F). The MCO is assumed to be a nominal 500 L (18 ft³). The initial hydrogen concentration is assumed to be 1% in the MCO. The initial pressure, at termination of vacuum and initiation of helium purge, is assumed to be 12 torr.

17.4 Software Applications

MATLAB software was utilized to plot the data generated from the analytical solutions (see EDT 626115).

17.5 Computer Model

Not applicable for this calculation.

17.6 Input Data

Bounding H ₂ generation rate:	2.4×10^{-3} g H ₂ /sec (Pajunen 1998)
MCO volume:	18 ft ³ (nominal 500 L) (Section 17.3)
MCO temperature:	50°C (Irwin et al 1999)
Initial MCO pressure:	12 torr (Section 17.3)

17.7 Calculations

Two solutions are required for determining the transient hydrogen concentration and pressure rise in the MCO after initiation of the helium purge. These modeling equations are developed in Appendix Q.

MCO pressure during helium purge:

$$P = \frac{RT}{V}(\alpha t + n^0) \quad (P-1)$$

where: P = MCO pressure during the helium purge, torr
 R = ideal gas constant, 62.36 (liter torr)/(mole K) or 0.04259 (psia-ft³)/(mole-K)
 T = MCO temperature, 323 K
 V = MCO volume, 500 L (18 ft³)
 n^0 = initial total moles of gas in the MCO equal to P^0V/RT , mole
 n_{H_2} = hydrogen generation rate, mole H₂/min
 n_{He} = helium ingress rate, mole He/min
 α = $n_{H_2} + n_{He}$, mol/min
 t = helium purge time, min

Hydrogen mole fraction in MCO during helium purge:

$$y_{H_2} = \frac{[n_{H_2} t + n^0 y^0]}{[\alpha t + n^0]} \quad (S-1)$$

where: y_{H_2} = hydrogen mole fraction in the MCO during helium purge
 y^0 = initial hydrogen mole fraction in the MCO

17.8 Results

Figure 17-1 displays the rising pressure under normal given input conditions at various helium purge rates. This figure shows it takes approximately 11 minutes to fill the MCO with the helium purge beginning at 12 torr and ending at 786 torr (0.5 psig). The minimum helium purge should be 3 SCFM or higher to meet these pressure limits within 5 minutes purge time.

Figure 17-2 shows the minimal helium purge rate at 1.4 SCFM to keep the hydrogen concentration below 4%. A helium purge rate of 6 SCFM or higher is required to maintain the MCO hydrogen concentration at 1% or lower.

17.9 Conclusions

Given the input parameters with the Bounding hydrogen generation rate, the plots demonstrate that the hydrogen concentration, pressure rise and associated "fill" time can be expected per a specific helium purge rate under normal conditions.

17.10 References

Boyce, W. E., and R. C. DiPrima, 1969, *Elementary Differential Equations and Boundary Value Problems, Second Edition*, John Wiley & Sons, Inc., New York, New York.

Irwin, J. J., C. R. Miska, S. A. Brisbin, C. C. Pitcoff, and R. Whitehurst, 1999, *Spent Nuclear Fuel Project Cold Vacuum Drying Facility Operations Manual*, SNF 2356, Rev. 1, DE&S Hanford, Incorporated, Richland, Washington

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

Figure 17-1 Transient Pressure Rise In The MCO At Various Helium Purge Rates. Bounding Hydrogen Generation Rate

Figure 17-2 Transient Hydrogen Concentration In The MCO During Various Helium Purge Rates. Bounding Hydrogen Generation Rate

18.0 Evaluation of Air In-leakage Criteria for Cold Vacuum Drying

18.1 Purpose and Objective

The purpose of this calculation is to document an earlier calculation of the allowable air in-leakage into an MCO through piping connections at the Cold Vacuum Drying Facility (CVDF).

18.2 Summary of Conclusions and Results

A design leak rate for piping systems connected to the MCO in the CVDF of 1×10^{-4} sccs (standard cubic centimeters per second) was selected based on preventing air ingress from interfering with the pressure rise measurement that supports the free water removal test procedure (pressure rise less than 2.4 torr/hr). The design leak rate results in a potential air ingress from mechanical connections to the MCO that is $1/4000^{\text{th}}$ of the gas generation rate corresponding to the pressure rise criterion.

18.3 Software Applications

Not applicable to this calculation.

18.4 Input Data

The following MCO operating conditions are used as a basis for the air in-leakage calculation based on Pajunen (1997):

Operating temperature:	50°C (323 K)
Operating pressure during pressure rebound test:	0.5 torr to 3 torr in 1 hr
MCO volume:	525 L

18.5 Calculation

The minimum quantity of gas entering an MCO that results in a pressure rise of 0.5 torr to 3 torr is calculated based on the ideal gas law (see Appendix R).

$$n = \frac{P V}{R T} = \frac{(3 - 0.5) \text{ torr/hr} \times 525 \text{ L}}{0.082 \text{ atm} \cdot \text{L/gmol} \cdot \text{K} \times 323 \text{ K} \times 760 \text{ torr/atm}} = 6.52 \times 10^{-2} \text{ gmol/hr} \quad (1)$$

The molar density of gas at standard conditions is:

$$\rho = \frac{n}{V} = \frac{P}{R T} = \frac{1 \text{ atm}}{0.082 \text{ atm} \cdot \text{L/gmol} \cdot \text{K} \times 273 \text{ K}} = 0.045 \text{ gmol/L} \quad (2)$$

Therefore, the volumetric leak rate at standard conditions that corresponds to the pressure rise criterion is:

$$\dot{V} = \frac{n}{\rho} = \frac{6.52 \times 10^{-2} \text{ gmol/hr} \times 1000 \text{ cc/L}}{0.045 \text{ gmol/L} \times 3600 \text{ sec/hr}} = 0.40 \text{ sccs} \quad (3)$$

18.6 Results

A leak rate criterion of 1×10^{-4} sccs is specified for the mechanical attachments to an MCO while being processed at the CVDF. This provides a design margin of 4000 (0.4/between the design leak criterion and a gas generation rate that fails the pressure rebound test criterion).

18.7 Conclusions

A leak rate specification of the pressure rise test criterion of 0.5 to 3 torr/hr in one hour was subsequently modified to 2.4 torr/hr in Pajunen, 1998. The modified pressure rise criterion does not significantly impact [changes the rate calculated by Equation (3) to 0.38 sccs] the conclusions of this calculation.

18.8 References

Pajunen, A. L., 1997, *Cold Vacuum Drying Process Technical Manual*, HNF-SD-SNF-TM-001, Rev 0, SGN Eurisys Services Corporation, Richland, Washington.

Pajunen, A. L., 1998, *Cold Vacuum Drying Residual Free Water Test Description*, HNF-1851, Rev 2, COGEMA Engineering Corporation, Richland, Washington.

19.0 Calculation of Hydrogen Concentrations During Air Ingress Events

19.1 Purpose and Objective

The purpose of this calculation is to identify the pressure of hydrogen which can exist in an MCO such that the hydrogen concentration does not exceed flammability limits during an air ingress event.

19.2 Summary of Conclusions and Results

The calculation concludes that an MCO starting with 12 torr of pure hydrogen will not develop gas mixtures that exceed flammability limits during an air ingress event. This initial condition results in a gas composition of 4 vol% hydrogen when the total system pressure is 300 torr. Therefore, if an event is postulated that starts with 12 torr of hydrogen and an air ingress occurs that stops at a total pressure of 300 torr, the gas mixture would be at the hydrogen flammability limit in air.

19.3 Assumptions

The flammability limit is assumed to vary linearly with total system pressure between the two data point observations described in Coward and Jones (1952). While it is unlikely that this type of relationship is strictly correct, the hydrogen concentration variation curves during an air ingress event are sufficiently less than the assumed flammability (see Figure 11-1) limit such that this assumption should not affect the conclusions of this calculation.

19.4 Software Applications

A spreadsheet (QUATTRO PRO[®] for Windows, Version 5.0) was used to produce graphs for this calculation.

19.5 Computer Model

Not applicable to this calculation.

19.6 Input Data

The hydrogen flammability limit in air variation with total system pressure is based on Coward and Jones (1952).

19.7 Calculations

19.7.1 Limit Data

Coward and Jones (1952) indicate the following data for the pressure dependence of flammability limits for hydrogen in air (see pg 17 of reference).

“Other experiments in narrow tubes (8, 16, and 25 mm. diameter), with upward propagation of flame, showed no great change in the limits until the pressure was below about 300 mm., when the range narrowed until below 50 mm no mixture propagated flame.”

This statement is interpreted to indicate that the flammability can be represented as a stoichiometric mixture of hydrogen in air when the total system pressure is 50 torr, and the hydrogen concentration at the flammability limit decreases to 4 vol% hydrogen in air as the system pressure increases to from 50 torr to 300 torr. Below 50 torr, no mixture of hydrogen in air is flammable and above 300 torr, to atmospheric pressure, the flammability limit is 4 vol%. This calculation assumes the lower flammability limit varies linearly with pressure between 50 torr and 300 torr.

Calculate stoichiometric hydrogen in air:

$$\text{Mol fraction H}_2 = \frac{P_H}{P_H + P_O + P_N} \quad (19-1)$$

where $P_{H,O,N}$ = partial pressure of hydrogen, oxygen, nitrogen

At stoichiometric conditions, $P_H = 2 P_O$, and $P_N = \left(\frac{P_O}{0.21}\right) (0.79)$, such that

$$\begin{aligned} \text{Mol fraction H}_2 &= \frac{2 P_O}{\left(2 + 1 + \frac{0.79}{0.21}\right) P_O} \\ &= 0.296 \end{aligned} \quad (19-2)$$

Therefore, the flammability limit is 29.6 vol% hydrogen at a total pressure of 50 torr and 4 vol% at a total pressure of 300 torr. A linear relationship between these points becomes:

$$\text{Slope} = \frac{\text{Vol\% H}_2 \text{ Limit}}{\text{Total System Pressure}} = \frac{(29.6 - 4)}{(50 - 300)} = -0.102 \frac{\text{vol\%}}{\text{torr}} \quad (19-3)$$

$$\begin{aligned} \text{Intercept} &= 29.6 - (-0.102)(50) = 34.7, \\ \text{or} &= 4 - (-0.102)(300) = 34.6 \end{aligned} \quad (19-4)$$

Based on the above, the following equations were used to model the pressure effect on the lower flammability limit for pressures below atmospheric.

$$\begin{aligned} \text{Vol\% H}_2 \text{ limit} &= \infty && \text{for } 50 \text{ torr} < P_{\text{total}} \\ \text{Vol\% H}_2 \text{ limit} &= 34.6 - (0.102) P_{\text{total}} && \text{for } 50 \text{ torr} \leq P_{\text{total}} \leq 300 \text{ torr} \\ \text{Vol\% H}_2 \text{ limit} &= 4 && \text{for } 300 \text{ torr} > P_{\text{total}} \geq 760 \text{ torr} \end{aligned} \quad (19-5)$$

19.7.2 Partial Pressure Hydrogen at Limits

The partial pressure of hydrogen at the two key limit points is calculate as follows:

$$P_H @ 50 \text{ torr limit} = (0.296) (50 \text{ torr}) = 14.8 \text{ torr} \quad (19-6)$$

$$P_H @ 300 \text{ torr limit} = (0.04) (300 \text{ torr}) = 12 \text{ torr} \quad (19-7)$$

Therefore, the 300 torr limit constrains the initial partial pressure of hydrogen which can be in an MCO at the start of an air ingress event. This can be illustrated by calculating the variation of hydrogen concentration in an MCO during an air ingress event start assuming alternative starting points of 12 or 14.8 torr of pure hydrogen in the system. The hydrogen concentration variation is calculated by the following equation.

$$\text{Vol\% H}_2 \text{ in system} = (100) \frac{P_{H,\text{initial}}}{P_{\text{total}}} \quad (19-8)$$

P_{total} increases from $P_{H,\text{initial}}$ to 760 torr as air leaks into an MCO.

19.8 Results

Figure 19-1 compares the MCO hydrogen concentration during an air ingress event starting from alternative initial pressures of hydrogen. Pure hydrogen is assumed at the start of the air ingress event. Starting at 14.8 torr hydrogen, the MCO hydrogen concentration passes through a region where the gas concentration exceeds the flammability limit when the total system pressure is near 300 torr. If the initial hydrogen pressure is 12 torr, the MCO hydrogen concentration is always maintained below the flammability limit during an air ingress event.

The margin for difference between the MCO gas concentration and the flammability limit depends on the final pressure established at the conclusion of the air ingress event. For a starting pressure of 12 torr, the MCO gas space composition would be just at the flammability limit if a final pressure of 300 torr was established at the conclusion of air ingress. The effect of reducing the starting pressure of hydrogen to 6 torr is shown on Figure 19-1 to indicate the margin that may be develop by selecting different hydrogen pressures at the start of an air ingress event.

19.9 Conclusions

Flammable gas mixtures can not be generated in an MCO by an air ingress event if the partial pressure of hydrogen is less than 12 torr at the time the air ingress event occurs.

19.10 References

Coward, H. F., and G. W. Jones, 1952, *Limits of Flammability of Gases and Vapors*, Bureau of Mines Bulletin 503, U. S. Department of the Interior, Washington, D. C.

Figure 19-1 Variation of hydrogen concentration in an MCO during an air ingress event.

20.0 “Non-Ideal” Mixing of Minimum Helium Purge to Reduce Hydrogen and Oxygen Concentrations in the MCO Void Space After a Vacuum Line Break

20.1 Purpose and Objectives

The purpose of this calculation is to determine that the helium purge design basis is adequate for controlling both the hydrogen concentration below 8.7% (Medsker et al 1999) [with “non-ideal” mixing of hydrogen, oxygen, and helium] and the oxygen concentration at or below 4% in the MCO void spaces after a vacuum line break. This section alters Section 12.0 (ideal mixing assumption).

20.2 Summary of Final Results and Conclusions

Overall mass (mole), air (thus, oxygen), and hydrogen balances were performed around the MCO void spaces (MCO void space model, mass balances and mathematical derivations attached in Appendix S). Numerical solutions were used to calculate the non-ideal mixing of hydrogen and air leak oxygen concentrations in the various void space sectors in an MCO.

Based on input parameters with a helium purge of 1.4 SCFM and a bounding hydrogen generation rate per each fuel and scrap basket, the hydrogen concentrations in the MCO void space sectors can always be maintained well below 8.7% and the oxygen concentrations can be maintained below 4%.

20.3 Assumptions

The vacuum line is assumed broken during the vacuum process, whereby, an initial condition assumes the MCO void space immediately fills with air at 1 atm. The broken vacuum line is assumed to be quickly shut off, with the MCO filled with air at 1 atm (0 psig), and the helium purge is assumed to immediately begin. The safety class exhaust valve is set at 10 psig. A bounding hydrogen generation rate is used. Helium gas (assumed 100% He) is used to purge the MCO. The initial H_2 concentration is assumed to be 2%. See Appendix S for the initial H_2 derivation. The hydrogen generation rates for the fuel and scrap baskets are calculated in Appendix S based on Pajunen (1998) and Reilly (1998).

The MCO gas is assumed to be “non-ideally” mixed due to the helium purge concentrating along the annulus void volumes and the fuel/scrap basket interference in each MCO. The model assumes each MCO is made up of 5 sectors for the MKIV MCOs and 6 sectors for the MKIA MCOs. Each sector is further assumed to consist of three separate void space sectors – Fuel or Scrap basket, Annulus, and Gap separating the fuel and/or scrap baskets. See Section Table 20-1 for void volumes in separate sectors with the H_2 and O_2 modeling (eight cases total). Each of these three void space sectors is assumed to be well-mixed. The helium flow is assumed to initiate the purge from the bottom of the MCO with 70% of the purge volume flowing through the fuel (or scrap) basket and the remaining 30% flowing through the annulus. No gap space exists in the bottom sector of the MCO with Cases 3 and 7 because 1 scrap basket is on the bottom and there is no gap space above it. Both flows are then combined in the gap void space leading to the next upper fuel/scrap basket and annulus. Figure 20-A presents a diagram of gas flows and volumes for the H_2 O_2 model.

Figure 20-A O₂ and H₂ Composition Model Per Sector

$i = 1$ through 6

20.4 Software Applications

MATLAB™ was used to solve and plot the Runge-Kutta (RK) numerical method results (see files in EDT 627108). Numerical solutions were used for the mass balance (both H₂ and O₂) derivations during both the increasing pressure and constant pressure (10 psig) portion of this problem with one exception - the first two O₂ balances around the bottom fuel/scrap basket were solved using an analytical method.

20.5 Computer Model

See Section 20.4 for modeling application and EDT 627108 for MATLAB plotting routines and Runge-Kutta subroutines. See Section 1.4 for time and pressure correlation used with MATLAB Runge-Kutta subroutine during the increasing pressure portion of this problem.

20.6 Input Data

Bounding H ₂ generation rate per MKIV Fuel Basket:	1.55×10^{-4} g H ₂ /sec (Appendix S)
Bounding H ₂ generation rate per MKIV Scrap Basket:	8.8×10^{-4} g H ₂ /sec (Appendix S)
Bounding H ₂ generation rate per MK1A Fuel Basket:	1.37×10^{-4} g H ₂ /sec (Appendix S)
Bounding H ₂ generation rate per MK1A Scrap Basket:	5.16×10^{-4} H ₂ /sec (Appendix S)
MCO void space volume:	See Table 20-1 (Praga 1998)
MCO void space temperature:	50°C (Irwin et al 1999a)
Initial MCO void space pressure:	14.7 psia (Section 20.3)
Final (Steady State) MCO void space pressure:	24.7 psia (10 psig)(Section 20.3)

The Standard Conditions (SC) associated with the helium ingress rate is taken to be:

Temperature, T = 0°C

Pressure, P = 14.7 psia

Table 20-1 lists the void volumes (total and per sector) for the eight different loading cases utilized in the oxygen model. The eight loading descriptions (max., max. part. load., and nominal) labeled in Table 20-1 designate the amount of void volume per case (Praga 1998). The basis for each case is reflective of the fuel type displacement, scrap displacement, and fuel basket displacement. Each case model is detailed, with void volumes, in Appendix S. The first portion of Table 20-1 displays the volume per sector with the number of sectors included in parenthesis (i.e., (5x)) to determine the total void volume of the specific void space in the MCO for each case. The second portion of Table 20-1 displays the volume percentage of the total void space in the MCO for each case.

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Table 20-1 Void Volumes Determined for O₂ Modeling

Fuel Type	MARK IV				MARK 1A			
	1	2	3	4	5	6	7	8
Case	1	2	3	4	5	6	7	8
Loading Description	Maximum Fuel Loading	Maximum Particulate Loading	Nominal Loading	Maximum Fuel Loading	Maximum Particulate Loading	Nominal Loading	Maximum Fuel Loading	Maximum Particulate Loading
No. Fuel Baskets	5	4	3	4	6	5	4	5
No. Scrap Baskets	0	1	2	1	0	1	2	1
Total Void Volume (L)	499	519	538	527	524	543	563	548
Annulus Void Volume (L)	(5x) 5.062	(5x) 5.005	(5x) 4.945	(5x) 5.082	(6x) 5.827	(6x) 5.632	(6x) 5.471	(6x) 5.684
Void Volume Between Fuel Baskets (L)	(4x) 36.101	(4x) 35.698	(3x) 35.267	(4x) 36.248	(5x) 29.563	(5x) 28.572	(4x) 27.756	(5x) 28.835
Void Volume Above Baskets (L)	60.395	24.022	23.732	24.343	65.225	45.217	54.368	46.633
Void Volume Scrap Baskets (L)	0.000	114.452	(2x) 113.070	116.217	0.000	98.838	(2x) 96.014	99.748
Void Volume Fuel Baskets (L)	(5x) 53.778	(4x) 53.177	(3x) 52.535	(4x) 53.997	(6x) 45.999	(5x) 44.458	(4x) 43.188	(5x) 44.868

Fuel Type	MARK IV				MARK 1A			
	1	2	3	4	5	6	7	8
Case	1	2	3	4	5	6	7	8
Loading Description	Maximum Fuel Loading	Maximum Particulate Loading	Nominal Loading	Maximum Fuel Loading	Maximum Particulate Loading	Nominal Loading	Maximum Fuel Loading	Maximum Particulate Loading
No. Fuel Baskets	5	4	3	4	6	5	4	5
No. Scrap Baskets	0	1	2	1	0	1	2	1
Total Void Volume (L)	499	519	538	527	524	543	563	548
Annulus Void Volume	5.1%	4.9%	4.6%	4.9%	6.8%	6.3%	5.9%	6.3%
Void Volume Between Fuel Baskets	29.2%	27.7%	19.8%	27.7%	28.6%	26.6%	19.9%	26.6%
Void Volume Above Baskets	12.2%	4.7%	4.4%	4.7%	12.6%	8.4%	9.7%	8.4%
Void Volume Scrap Baskets	0.0%	22.2%	42.2%	22.2%	0.0%	18.4%	34.4%	18.4%
Void Volume Fuel Baskets	53.5%	40.6%	29.0%	40.6%	52.0%	40.3%	30.2%	40.3%

20.7 Calculations

The modeling equation solutions are divided into two parts for both the oxygen and hydrogen mass balances. The first part involves the helium purge after the vacuum line break and succeeding increased MCO pressure from 1 atm (0 psig) to the opening of the safety class valve at 10 psig. The second part involves the constant pressure helium purge at 10 psig. These modeling equations are developed in Appendix S.

The modeling equations used in the O₂ analysis use subscript A, B, and C to designate the fuel/scrap basket void space, the annulus, and the gap between the baskets, respectively.

Increasing Pressure Portion in the 6 MCO Sectors

1st Sector – O₂ mole fraction

Air mole fraction in the 1st Fuel/Scrap basket void space during pressure rise from 0 to 10 psig:

$$y_{A1} = y_{A1}^0 \left[n_{A1}^0 / (\alpha_{A1} t + n_{A1}^0) \right]^{\gamma_{A1} + 1} \quad \text{Fuel/Scrap Basket \#1}$$

where: y_{A1} = air mole fraction in the 1st fuel/scrap basket void space during pressure rise

y_{A1}^0 = initial air mole fraction in the 1st fuel/scrap basket void space

V_{A1} = void space volume of the 1st fuel/scrap basket, ft³ – See Table 20-1 for volume

V_{mco} = void space volume of the MCO, ft³ – See Table 20-1 for volume

P^0 = initial MCO void space pressure, 14.7 psia

T = temperature of the MCO gas, 323 K

R = ideal gas constant, 0.04259 (psia-ft³)/(mole-K)

n_{He} = helium ingress rate, mole He/min

n_{H2} = hydrogen generation rate, mole H₂/min (note: this rate depends on if basket is scrap or fuel)

n_{A1}^0 = initial moles of gas in the 1st fuel/scrap basket void space, $P^0 V_{A1} / RT$, mole

n_{H2} MCO total = total hydrogen generation rate in MCO, mol H₂/min

$\alpha = n_{H2}$ MCO total + n_{He} , mole/min

$\alpha_{A1} = (V_{A1}/V_{mco}) \alpha$, mole/min

$\gamma_{A1} = [n_{H2} + 0.70(n_{He}) - (V_{A1}/V_{mco}) \alpha] / n_{H2}$

t = helium purge time after vacuum line break, min

Therefore, the oxygen mole fraction, assumed 21% of air, in the MCO Fuel/Scrap basket void space is:

$$y_{O_2 A1} = 0.21 y_{A1}$$

Air mole fraction in the 1st Annulus void space during pressure rise from 0 psig to 10 psig:

$$y_{B1} = y_{B1}^0 \left[n_{B1}^0 / (\alpha_{B1} t + n_{B1}^0) \right]^{\gamma_{B1} + 1} \quad \text{Annulus \#1}$$

where: y_{B1} = air mole fraction in the 1st Annulus void space during pressure rise
 y_{B1}^0 = initial air mole fraction in the 1st Annulus void space
 V_{B1} = void space volume of the 1st Annulus, ft³ - See Table 20-1 for volume
 n_{B1}^0 = initial moles of gas in the 1st Annulus void space, $P^0 V_{B1} / RT$, mole
 $\alpha_{B1} = (V_{B1} / V_{mco}) \alpha$, mole/min
 $\gamma_{B1} = [n_{H2} + 0.30(n_{He}) - (V_{B1} / V_{mco}) \alpha] / n_{H2}$

Therefore, the oxygen mole fraction, assumed 21% of air, in the Annulus void space is:

$$y_{O_2 B1} = 0.21 y_{B1}$$

Air mole fraction in the 1st Gap void space during pressure rise from 0 to 10 psig cannot easily be solved analytically, therefore the ordinary differential equation set up for the numerical solver is:

$$\frac{dy_{C1}}{dt} = (1/n_{C1}) \left[n_{F1} y_{A1} + n_{G1} y_{B1} - n_{EX1} y_{C1} - \alpha_{C1} y_{C1} \right] \quad \text{Gap \#1}$$

where: y_{C1} = air mole fraction in the 1st gap void space during pressure rise
 n_{EX1} = (exit gas from gap 1 - See EDT 627108 for value), mole He/min
 $n_{C1} = (P V_{C1} / RT)$, mole gas in 1st gap void space
 $n_{F1} = n_{H2} + A_{flow} (n_{He}) - (V_{C1} / V_{mco}) \alpha$, mole/min
 $n_{G1} = n_{D1} - (V_{B1} / V_{mco}) \alpha$, mole/min
 $n_{D1} = B_{flow} (n_{He})$, mole/min
 V_{C1} = void space volume of the 1st gap void space, ft³ - See Table 20-1 for volume
 $\alpha = 6 n_{H2} + n_{He}$, mole/min (note: 6 is replaced with 5 if MKIA MCO)
 $\alpha_{C1} = (V_{C1} / V_{mco}) \alpha$, mole/min

2nd Sector - O₂ mole fraction

$$\frac{dy_{A2}}{dt} = (1/n_{A2}) \left[n_{E2} y_{C1} - \alpha_{A2} y_{A2} - n_{F2} y_{A2} \right] \quad \text{Fuel Basket \#2}$$

where: y_{A2} = air mole fraction in the 2nd Fuel basket void space during pressure rise
 $n_{A2} = (P V_{A2} / RT)$, mole gas in 2nd Fuel basket
 $n_{E2} = 0.70 n_{EX1}$ (split exit gas from gap 2), mole He/min
 $n_{F2} = n_{H2} + 0.70 (n_{EX1}) - (V_{A2} / V_{mco}) \alpha$, mole/min
 V_{A2} = void space volume of the 2nd Fuel basket, ft³ - See Table 20-1 for volume
 $\alpha_{A2} = (V_{A2} / V_{mco}) \alpha$, mole/min

$$\frac{dy_{B2}}{dt} = (1/n_{B2})[n_{D2} y_{C1} - \alpha_{B2} y_{B2} - n_{G2} y_{B2}] \quad \text{Annulus \#2}$$

where: y_{B2} = air mole fraction in the 2nd Annulus void space during pressure rise
 n_{B2} = (PV_{B2}/RT) , mole gas in 2nd Annulus void space, mole
 n_{D2} = $0.30n_{EX1}$ (split exit gas from gap 2), mole He/min
 n_{G2} = $n_{D2} - (V_{B2}/V_{mco}) \alpha$, mole/min
 V_{B2} = void space volume of the 2nd Annulus, ft³ - See Table 20-1 for volume
 α_{B2} = $(V_{B2}/V_{mco}) \alpha$, mole/min

$$\frac{dy_{C2}}{dt} = (1/n_{C2})[n_{F2} y_{A2} + n_{G2} y_{B2} - n_{EX2} y_{C2} - \alpha_{C2} y_{C2}] \quad \text{Gap \#2}$$

where: y_{C2} = air mole fraction in the 2nd gap void space during pressure rise
 n_{C2} = (PV_{C2}/RT) , mole gas in 2nd gap void space
 n_{EX2} = (exit gas from gap 2 - See EDT 627108 for value), mole He/min
 n_{F2} = $n_{H2} + 0.70 (n_{He}) - (V_{C2}/V_{mco}) \alpha$, mole/min
 n_{D2} = $0.30 (n_{He})$, mole/min
 V_{C2} = void space volume of the 2nd gap void space, ft³ - See Table 20-1 for volume
 α_{C2} = $(V_{C2}/V_{mco}) \alpha$, mole/min

Note: For the remaining expressions (#3 through #6) see Appendix S for subscripted values.

3rd Sector - O₂ mole fraction

$$\frac{dy_{A3}}{dt} = (1/n_{A3})[n_{E3} y_{C2} - \alpha_{A3} y_{A3} - n_{F3} y_{A3}] \quad \text{Fuel Basket \#3}$$

$$\frac{dy_{B3}}{dt} = (1/n_{B3})[n_{D3} y_{C2} - \alpha_{B3} y_{B3} - n_{G3} y_{B3}] \quad \text{Annulus \#3}$$

$$\frac{dy_{C3}}{dt} = (1/n_{C3})[n_{F3} y_{A3} + n_{G3} y_{B3} - n_{EX3} y_{C3} - \alpha_{C3} y_{C3}] \quad \text{Gap \#3}$$

4th Sector - O₂ mole fraction

$$\frac{dy_{A4}}{dt} = (1/n_{A4})[n_{E4} y_{C3} - \alpha_{A4} y_{A4} - n_{F4} y_{A4}] \quad \text{Fuel Basket \#4}$$

$$\frac{dy_{B4}}{dt} = (1/n_{B4})[n_{D4} y_{C3} - \alpha_{B4} y_{B4} - n_{G4} y_{B4}] \quad \text{Annulus \#4}$$

$$\frac{dy_{C4}}{dt} = (1/n_{C4})[n_{F4} y_{A4} + n_{G4} y_{B4} - n_{EX4} y_{C4} - \alpha_{C4} y_{C4}] \quad \text{Gap \#4}$$

5th Sector – O₂ mole fraction

$$\frac{dy_{A5}}{dt} = (1/n_{A5})[n_{E5} y_{C4} - \alpha_{A5} y_{A5} - n_{F5} y_{A5}] \quad \text{Fuel/Scrap Basket \#5}$$

$$\frac{dy_{B5}}{dt} = (1/n_{B5})[n_{D5} y_{C4} - \alpha_{B5} y_{B5} - n_{G5} y_{B5}] \quad \text{Annulus \#5}$$

$$\frac{dy_{C5}}{dt} = (1/n_{C5})[n_{F5} y_{A5} + n_{G5} y_{B5} - n_{EX5} y_{C5} - \alpha_{C5} y_{C5}] \quad \text{Gap \#5}$$

Note: In the last expression above (Gap #5), set $n_{EX5} = 0$ for an MCO with only 5 baskets

6th Sector – O₂ mole fraction

$$\frac{dy_{A6}}{dt} = (1/n_{A6})[n_{E6} y_{C5} - \alpha_{A6} y_{A6} - n_{F6} y_{A6}] \quad \text{Fuel/Scrap Basket \#6}$$

$$\frac{dy_{B6}}{dt} = (1/n_{B6})[n_{D6} y_{C5} - \alpha_{B6} y_{B6} - n_{G6} y_{B6}] \quad \text{Annulus \#6}$$

$$\frac{dy_{C6}}{dt} = (1/n_{C6})[n_{F6} y_{A6} + n_{G6} y_{B6} - \alpha_{C6} y_{C6}] \quad \text{Gap \#6}$$

Special case 3 and 7 (with bottom scrap basket)

Air mole fraction around 2nd tier fuel basket (above scrap basket) during changing pressure.

$$\frac{dy_{A2}}{dt} = \frac{1}{n_{A2}}[n_{F1} y_{A1} - n_{F2} y_{A2} - \alpha_{A2} y_{A2}]$$

Air mole fraction around 2nd Annulus (with bottom scrap basket) during changing pressure

$$\frac{dy_{B2}}{dt} = \frac{1}{n_{B2}}[n_{E1} y_{B1} - n_{G2} y_{B2} - \alpha_{B2} y_{B2}]$$

Air mole fraction around 2nd tier fuel basket (above scrap basket) at constant pressure of 10 psig

$$\frac{dy_{A2}}{dt} = \frac{1}{n_{A2}}[n_{F1} y_{A1} - n_{F2} y_{A2}]$$

Air mole fraction around 2nd Annulus (with bottom scrap basket) at constant pressure of 10 psig

$$\frac{dy_{B2}}{dt} = \frac{1}{n_{B2}} [n_{E1}y_{B1} - n_{G2}y_{B2}]$$

Constant Pressure Portion in the 6 MCO Sectors

1st Sector – O₂ mole fraction

Air mole fraction in the 1st Fuel/Scrap basket void space during a constant pressure of 10 psig:

$$\frac{dy_{A1}}{dt} = \frac{-n_{F1}}{n_{A1}} y_{A1}$$

Air mole fraction in the 1st Annulus void space during a constant pressure of 10 psig:

$$\frac{dy_{B1}}{dt} = \frac{-n_{G1}}{n_{B1}} y_{B1}$$

Air mole fraction in the 1st Gap void space during a constant pressure of 10 psig:

$$\frac{dy_{C1}}{dt} = \frac{1}{n_{C1}} [n_{F1}y_{A1} + n_{G1}y_{B1} - n_{EX1}y_{C1}]$$

2nd through 6th Sectors – ($i = 2$ to 6) for MKIV Fuel and 2nd through 5th Sectors ($i = 2$ to 5) for MK1A Fuel

Air mole fraction in the i^{th} Fuel basket void space during a constant pressure of 10 psig:

$$\frac{dy_{Ai}}{dt} = \frac{1}{n_{Ai}} [n_{Ei}y_{C(i-1)} - n_{Fi}y_{Ai}]$$

Air mole fraction in the i^{th} Annulus void space during a constant pressure of 10 psig:

$$\frac{dy_{Bi}}{dt} = \frac{1}{n_{Bi}} [n_{Bi}y_{C(i-1)} - n_{Gi}y_{Bi}]$$

Air mole fraction in the i^{th} Gap void space during a constant pressure of 10 psig:

$$\frac{dy_{Ci}}{dt} = \frac{1}{n_{Ci}} [n_{Fi}y_{Ai} + n_{Gi}y_{Bi} - n_{EXi}y_{Ci}]$$

Increasing Pressure Portion in the 6 MCO Sectors

1st Sector – H₂ mole fraction

Hydrogen mole fraction in the 1st Fuel/Scrap Basket void space during pressure rise from 0 to 10 psig:

Note: y_1 represents in the following section the H₂ mole fraction, NOT the O₂

$$\frac{dy_{A1}}{dt} = \frac{1}{n_{A1}} [n_{H2} - n_{F2}y_{A1} - \alpha_{A1}y_{A1}]$$

Hydrogen mole fraction in the 1st Annulus void space during the pressure rise from 0 to 10 psig:

$$\frac{dy_{B1}}{dt} = \frac{-1}{n_{B1}} [n_{E1}y_{B1} + \alpha_{B1}y_{B1}]$$

Hydrogen mole fraction in the 1st Gap void space during the pressure rise from 0 to 10 psig:

$$\frac{dy_{C1}}{dt} = \frac{1}{n_{C1}} [n_{F1}y_{A1} + n_{G1}y_{B1} - n_{EX1}y_{C1} - \alpha_{C1}y_{C1}]$$

Hydrogen mole fraction in the 2nd through 6th Sectors ($i = 2$ to 6) for MKIV Fuel and 2nd through 5th Sectors ($i = 2$ to 5) for MK1A fuel

5th Fuel/Scrap Basket void space during changing pressure

$$\frac{dy_{Ai}}{dt} = \frac{1}{n_{Ai}} [n_{H2} + n_{Ei}y_{C(i-1)} - n_{Fi}y_{Ai} - \alpha_{Ai}y_{Ai}]$$

5th Annulus void space during changing pressure

$$\frac{dy_{Bi}}{dt} = \frac{1}{n_{Bi}} [n_{Di}y_{C(i-1)} - n_{Gi}y_{Bi} - \alpha_{Bi}y_{Bi}]$$

i^{th} Gap void space during changing pressure

$i = 1$ to 4 for MCIV Fuel

$i = 1$ to 5 for MK1A Fuel

$$\frac{dy_{Ci}}{dt} = \frac{1}{n_{Ci}} [n_{Fi}y_{Ai} + n_{Gi}y_{Bi} - n_{EXi}y_{Ci} - \alpha_{Ci}y_{Ci}]$$

and for $i = 5$ for MKIV Fuel (top gap void space)
 $i = 6$ for MK1A Fuel (top gap void space)

$$\frac{dy_{Ci}}{dt} = \frac{1}{n_{Ci}} [n_{Fi} y_{Ai} + n_{Gi} y_{Bi} - \alpha_{Ci} y_{Ci}]$$

Special case 3 and 7 (with bottom Scrap Basket)

H₂ mole fraction around 2nd tier Fuel Basket (above Scrap Basket) during changing pressure:

$$\frac{dy_{A2}}{dt} = \frac{1}{n_{A2}} [n_{F1} y_{A1} + n_{H2} - n_{F2} y_{A2} - \alpha_{A2} y_{A2}]$$

H₂ mole fraction around 2nd Annulus (above Scrap Basket) during changing pressure:

$$\frac{dy_{B2}}{dt} = \frac{1}{n_{B2}} [n_{G1} y_{B1} - n_{G2} y_{B2} - \alpha_{B2} y_{B2}]$$

Hydrogen mole fraction in the 1st Gap void space during constant pressure at 10 psig:

1st Fuel/Scrap Basket void space

$$\frac{dy_{A1}}{dt} = \frac{1}{n_{A1}} [n_{H2} - n_{F1} y_{A1}]$$

1st Annulus void space

$$\frac{dy_{B1}}{dt} = \frac{-n_{G1}}{n_{B1}} y_{B1}$$

1st Gap Void space

$$\frac{dy_{C1}}{dt} = \frac{1}{n_{C1}} [n_{F1} y_{A1} + n_{G1} y_{B1} - n_{EX1} y_{C1}]$$

Hydrogen mole fraction in the 2nd through 6th Sectors ($i = 2$ to 6) for MKIV Fuel and 2nd through 5th Sectors ($i = 2$ to 5) for MK1A Fuel

5th Fuel/Scrap Basket void space at constant pressure:

$$\frac{dy_{Ai}}{dt} = \frac{1}{n_{Ai}} [n_{H2} + n_{Ei} y_{C(i-1)} - n_{Gi} y_{Ai}]$$

i^{th} Annulus void space at constant pressure:

$$\frac{dy_{Bi}}{dt} = \frac{1}{n_{Bi}} [n_{Di} y_{C(i-1)} - n_{Gi} y_{Bi}]$$

i^{th} Gap void space at constant pressure:

$$\frac{dy_{Ci}}{dt} = \frac{1}{n_{Ci}} [n_{Fi} y_{Ai} + n_{Gi} y_{Bi} - n_{Ei} y_{Ci}]$$

Special Case 3 and 7 (with bottom Scrap Basket)

H₂ mole fraction around 2nd tier Fuel Basket (above Scrap Basket) at constant pressure:

$$\frac{dy_{A2}}{dt} = \frac{1}{n_{B2}} [n_{G1} y_{B1} - n_{G2} y_{B2}]$$

20.8 Results

An analysis using non-ideal mixing of the helium purge flow is presented in 8 cases representing the MCO fuel type and loading. Figures 20-45 through 20-88 show the hydrogen concentrations in the different MCO sectors (i.e., Fuel/Scrap basket void space, Annulus, and Gap) for the eight cases. Case 3 (Figure 20-59) shows the highest concentration of hydrogen gas in the top scrap basket reaches just over 4% after approximately four to five minutes of helium purge time. Figures 20-1 through 20-44 show the oxygen concentrations in the different MCO sectors for the eight cases. Case 3 (Figure 20-15) show the longest purge time takes approximately 27 minutes to reach 4% O₂ in the top scrap basket.

20.9 Conclusions

Given the input parameters with the bounding hydrogen generation rate, the plots demonstrate that the hydrogen and oxygen concentrations in the MCO void sectors, after an air ingress leak, can be maintained indefinitely below 8% and 4%, respectively, with a minimum helium purge rate of 1.4 SCFM.

20.10 References

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Figure 20-1 Case 1: 5 Fuel Baskets - Transient O₂ Concentrations in MKIV MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-2 Case 1: 5 Fuel Baskets - Transient O₂ Concentrations in MKIV MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-3 Case 1: 5 Fuel Baskets - Transient O₂ Concentrations in MKIV MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-4 Case 1: 5 Fuel Baskets - Transient O₂ Concentrations in MKIV MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-5 Case 1: 5 Fuel Baskets - Transient O₂ Concentrations in MKIV MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-6 Case 2: 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-7 Case 2: 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-8 Case 2: 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-9 Case 2: 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-10 Case 2: 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-11 Case 3: 3 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MKIV MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-12 Case 3: 3 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MKIV MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-13 Case 3: 3 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MKIV MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-14 Case 3: 3 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MKIV MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-15 Case 3: 3 Fuel Baskets and 2 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-16 Case 4: Nominal - 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-17 Case 4: Nominal - 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-18 Case 4: Nominal - 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-19 Case 4: Nominal - 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-20 Case 4: Nominal - 4 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MKIV MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-21 Case 5: 6 Fuel Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-22 Case 5: 6 Fuel Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-23 Case 5: 6 Fuel Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-24 Case 5: 6 Fuel Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-25 Case 5: 6 Fuel Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-26 Case 5: 6 Fuel Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #6 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-27 Case 6: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-28 Case 6: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-29 Case 6: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-30 Case 6: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-31 Case 6: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-32 Case 6: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #6 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-33 Case 7: 4 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-34 Case 7: 4 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-35 Case 7: 4 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-36 Case 7: 4 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-37 Case 7: 4 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-38 Case 7: 4 Fuel Baskets and 2 Scrap Baskets - Transient O₂ Concentrations in MK1A MCO Void Sector #6 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-39 Case 8: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-40 Case 8: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-41 Case 8: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-42 Case 8: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-43 Case 8: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-44 Case 8: 5 Fuel Baskets and 1 Scrap Basket - Transient O₂ Concentrations in MK1A MCO Void Sector #6 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-45 Case 1: 5 Fuel Baskets - Transient H_2 Concentrations in MKIV MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-46 Case 1: 5 Fuel Baskets – Transient H_2 Concentrations in MKIV MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-47 Case 1: 5 Fuel Baskets – Transients H_2 Concentrations in MKIV MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-48 Case 1: 5 Fuel Baskets – Transient H_2 Concentrations in MKIV MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-49 Case 1: 5 Fuel Baskets – Transient H_2 Concentrations in MKIV MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate

Figure 20-50 Case 2: 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 2-51 Case 2: 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-52 Case 2: 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-53 Case 2: 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-54 Case 2: 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-55 Case 3: 3 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MKIV MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-56 Case 3: 3 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MKIV MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-57 Case 3: 3 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MKIV MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-58 Case 3: 3 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MKIV MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-59 Case 3: 3 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MKIV MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-60 Case 4: Nominal – 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-61 Case 4: Nominal – 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-62 Case 4: Nominal – 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-63 Case 4: Nominal – 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-64 Case 4: Nominal – 4 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MKIV MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-65 Case 5: 6 Fuel Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-66 Case 5: 6 Fuel Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-67 Case 5: 6 Fuel Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-68 Case 5: 6 Fuel Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-69 Case 5: 6 Fuel Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-70 Case 5: 6 Fuel Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #6 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-71 Case 6: 5 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MK1A MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-72 Case 6: 5 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MK1A MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-73 Case 6: 5 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MK1A MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-74 Case 6: 5 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MK1A MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-75 Case 6: 5 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MK1A MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-76 Case 6: 5 Fuel Baskets and 1 Scrap Basket – Transient H_2 Concentrations in MK1A MCO Void Sector #6 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-77 Case 7:4 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-78 Case 7: 4 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-79 Case 7: 4 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-80 Case 7: 4 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-81 Case 7: 4 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-82 Case 7: 4 Fuel Baskets and 2 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #6 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-83 Case 8: 5 Fuel Baskets and 1 Scrap Baskets – Transient H₂ Concentrations in MK1A MCO Void Sector #1 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-84 Case 8: 5 Fuel Baskets and 1 Scrap Baskets – Transient H₂ Concentrations in MK1A MCO Void Sector #2 During Helium Purge After Vacuum Line Break. Bounding H₂ Generation Rate.

Figure 20-85 Case 8: 5 Fuel Baskets and 1 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #3 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-86 Case 8: 5 Fuel Baskets and 1 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #4 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-87 Case 8: 5 Fuel Baskets and 1 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #5 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

Figure 20-88 Case 8: 5 Fuel Baskets and 1 Scrap Baskets – Transient H_2 Concentrations in MK1A MCO Void Sector #6 During Helium Purge After Vacuum Line Break. Bounding H_2 Generation Rate.

21.0 Calculation of Minimum Helium Purge

21.1 Purpose and Objective

The purpose of this calculation is to identify the minimum helium purge rate during an MCO steady state helium purge operation such that the hydrogen concentration does not exceed flammability limits. Calculations are performed for cases using both ideal and non-ideal mixing assumptions.

21.2 Summary of Conclusions and Results

The calculation concludes that an MCO will not develop gas mixtures that exceed flammability limits during a steady state minimum helium purge operation. The minimum MCO steady state helium purge has been calculated to be 0.7 SCFM with an established H₂ criteria limit of less than 8.7 % H₂ concentration in helium prior to mixing with air (Medsker et al 1999).

21.3 Assumptions

The helium purge gas is assumed, at actual conditions, to be 70°F (294K) at a pressure of 1 atm. Also included is the assumption of helium purge gas, at standard conditions, to be 32°F (273K) at a pressure of 1 atm. Both MCO helium purge conditions are assumed to be at steady state (constant total moles and constant H₂ concentration throughout the purge).

21.4 Software Applications

Not applicable to this calculation.

21.5 Computer Model

Not applicable to this calculation.

21.6 Input Data

Ideal Case

Bounding H₂ generation rate: 2.4×10^{-3} g H₂/sec (Pajunen 1998)

Non-Ideal Case

Bounding H ₂ generation rate per MKIV Fuel Basket:	1.55×10^{-4} g H ₂ /sec (Appendix S)
Bounding H ₂ generation rate per MKIV Scrap Basket:	8.8×10^{-4} g H ₂ /sec (Appendix S)
Bounding H ₂ generation rate per MK1A Fuel Basket:	1.37×10^{-4} g H ₂ /sec (Appendix S)
Bounding H ₂ generation rate per MK1A Scrap Basket:	5.16×10^{-4} H ₂ /sec (Appendix S)

The conditions associated with the helium ingress rate are taken to be:

Actual Conditions (AC):

Temperature, $T_{AC} = 70^{\circ}\text{F}$ (294K)

Pressure, $P = 1 \text{ atm}$ (14.696 psia)

Standard Conditions (SC):

Temperature, $T_{SC} = 32^{\circ}\text{F}$ (273K)

Pressure, $P = 1 \text{ atm}$ (14.696 psia)

21.7 Calculations

Ideal Mixing*in* : $\dot{n}_{h_2}$ *out* : $\dot{n}_{exy}$ **where y is the hydrogen gas fraction**

$$\text{Accum: } \frac{d(ny)}{dt} = 0 \quad \frac{dn}{dt} = 0 \quad \frac{dy}{dt} = 0 \quad H_2 \text{ concentration not changing and gmol gas in MCO not changing}$$

$$\therefore \dot{n}_{h_2} = \dot{n}_{exy}$$

$$\therefore y = \frac{\dot{n}_{h_2}}{\dot{n}_{ex}} = \frac{\dot{n}_{h_2}}{\dot{n}_{h_2} + \dot{n}_{he}}$$

find $\dot{V}_{sc}$ helium : set $y = 0.087$

$$\dot{n}_{he} = \frac{P_{sc} \dot{V}_{sc}}{RT_{sc}}$$

$$\therefore n_{h_2} + n_{he} = \frac{n_{h_2}}{y} \quad \text{or} \quad n_{he} = \frac{n_{h_2}}{y} - n_{h_2} = n_{h_2} \left(\frac{1}{y} - 1 \right)$$

$$\frac{P_{sc} \dot{V}_{sc}}{R T_{sc}} = n_{h_2} \left(\frac{1}{y} - 1 \right)$$

$$\therefore \dot{V}_{sc} = \frac{\dot{n}_{h_2} R T_{sc}}{P_{sc}} \left(\frac{1}{y} - 1 \right) \quad [\text{scfm}]$$

$$\dot{n}_{h_2} = 0.072 \text{ gmol } H_2 / \text{min} \quad P_{sc} = 14.696 \text{ psia}$$

$$R = 0.04259 \frac{\text{psia} \cdot \text{ft}^3}{\text{gmol} \cdot \text{K}} \quad T_{sc}(70^\circ F) = 294 K$$

$$H_2 \text{ limit} \rightarrow y = 0.087$$

$$\therefore \dot{V}_{sc} = \frac{\left(0.072 \frac{\text{gmol } H_2}{\text{min}} \right) \left(0.04259 \frac{\text{psia} \cdot \text{ft}^3}{\text{gmol} \cdot \text{K}} \right) (294 K)}{(14.696 \text{ psia})} \left(\frac{1}{0.087} - 1 \right) = 0.644 \frac{\text{ft}^3}{\text{min}}$$

$$\text{and with } T_{sc} = 273 K,$$

$$\therefore \dot{V}_{sc} = 0.644 \left(\frac{273 K}{294 K} \right) = 0.598 \frac{\text{ft}^3}{\text{min}}$$

$$\therefore \text{conservative to set } \dot{V}_{sc} = 0.7 \text{ CFM}$$

Non-Ideal Mixing

The non-ideal mixing model presented in Section 20.0 was used for an MCO containing two scrap baskets, assuming a helium purge flow rate of 0.7 SCFM to verify that transient hydrogen concentrations do not exceed 8.7% at some point in the MCO when purged with this minimum flow rate. The bounding cases from Section 20.0 for hydrogen concentrations were used.

Figure 21-1 Case 3: Transient H₂ Concentrations using “Non-Ideal” Modeling With A Helium Purge at 0.7 SCFM. Bounding H₂ Generation.

Figure 21-2 Case 7: Transient H₂ Concentrations using “Non-Ideal” Modeling With A Helium Purge at 0.7 SCFM. Bounding H₂ Generation.

21.8 Results

The calculation concludes that an MCO will not develop gas mixtures that exceed flammability limits during a steady state minimum helium purge flow of 0.7 SCFM.

Figure 21-1 and Figure 21-2 show the H₂ concentrations utilizing the "non-ideal" modelling equations from Section 20 at a helium flow of 0.7 SCFM. Case 3 and Case 7 each have two scrap baskets included in these MCOs for MKIV and MIA fuel, respectively. These two cases have been shown to generate the highest concentration of hydrogen in the MCO void spaces in Section 20.0. Transient calculations show that both MCOs are maintained below 8.7% hydrogen by a helium purge of 0.7 SCFM.

21.9 Conclusions

Flammable gas mixtures are not generated in an MCO under steady state operation with minimal helium purge greater than or equal to 0.7 SCFM.

21.10 References

Medsker, M. A., M. R. Piepho, and P. R. Rittman, 1999, *Cold Vacuum Drying Facility Design Basis Accident Analysis Documentation*, SNF-2770, Rev. 3, Fluor Daniel Northwest, Incorporated, Richland, Washington.

Pajunen, A. L., 1998, *Design Basis for Hydrogen Generation in the Cold Vacuum Drying Facility*, HNF-2458, Rev. 0A, COGEMA Engineering Corporation, Richland, Washington.

22.0 Evaluation of Adequate Safety Class Helium Gas Bottle Pressure

22.1 Purpose and Objectives

The purpose of this calculation is to ensure the CVDF safety class helium gas bottle pressure is adequate for a 30-minute MCO helium purge at 3.6 SCFM flow.

22.2 Summary of Final Results and Conclusions

An initial required gas bottle pressure of 1540 psig is calculated for a constant gas temperature of 115°F with a remaining pressure heel of 200 psig in the helium bottle.

22.3 Assumptions

The Benedict-Webb-Rubin (B-W-R) equation of state is utilized since a high pressure is involved. A minimum bottle pressure (heel) required after the 30-minute purge is assumed to be 200 psig. Helium flow is assumed to be 3.6 SCFM. The 3.6 SCFM assumption is based on an approximate 10% increase above the maximum flow through the system, under any condition, of 3.2 SCFM (Heard 1999); therefore, 3.6 SCFM is bounding when estimating how long the helium gas bottle lasts.

22.4 Software Applications

MATLAB software was utilized to determine both a 'trial and error' and final solution with the B-W-R equation of state (see EDT 627108).

22.5 Computer Model

Not applicable to this calculation.

22.6 Input Data

Helium ingress rate:	3.6 SCFM (Section 22.3)
Helium gas bottle temperature:	115°F (Section 22.3)
Helium gas bottle volume:	43.2 L (1.526 ft ³) (Matheson Model No. 1A (93-113-01))

The Standard Conditions (SC) associated with the helium ingress rate are taken to be:
Temperature, $T = 273$ K
Pressure, $P = 14.7$ psia

See Section 22.3 and EDT 627108 for input data.

22.7 Calculations

To calculate the required number of moles of helium gas in bottle after 30 minutes of purge:

$$n_{\text{He}} = \left(\frac{P\dot{V}}{RT} \right)_{\text{SC}} t = 136.5 \text{ moles}$$

where: n_{He} = total helium gas, moles

P = standard pressure, 14.696 psia (1 atm)

R = ideal gas constant, 0.04259 (psia-ft³)/(gmol-K)

T = 273K

$\dot{V}$ = helium gas bottle flow, 3.6 SCFM

t = total helium purge time, 30 min

The number of moles of helium gas required for a minimum pressure of 200 psig remaining in the gas bottle after the 30 minute purge is first calculated using a trial-and-error method utilizing the B-W-R equation of state at P equal to 200 psig (see B-W-R equation below). The number of moles of helium (n_{He}) remaining in the tank at 115°F is calculated to be approximately 24 moles. The gas bottle pressure is derived by adding the initial moles of gas to the 30-minutes purge gas moles (136.5 moles) and solving for P in the gas bottle at each temperature using the B-W-R equation of state.

B-W-R equation of state (Hsieh 1975):

$$P = \frac{RT}{V/n_{\text{He}}} + \left(B_0 RT - A_0 - \frac{C_0}{T^2} \right) \frac{1}{(V/n_{\text{He}})^2} + (bRT - a) \frac{1}{(V/n_{\text{He}})^3} + \frac{a\alpha}{(V/n_{\text{He}})^6} + \frac{c(1 + \gamma/(V/n_{\text{He}})^2)}{T^2} \frac{1}{(V/n_{\text{He}})^3} e^{-\gamma/(V/n_{\text{He}})}$$

where: n = moles of helium, 160.3 mol He

V = helium gas bottle volume, 43.2 liters

R = 0.08206 (atm-liter)/(mol-K)

T = helium gas bottle, 289 K (60°F), 308 K (95°F), and 319 K (115°F)

A_0 = 0.040962 (atm-liter²)/mol²

B_0 = 0.023661 liter/mol

C_0 = -1.6227e-13 (atm-K²-liter²)/mol

a = -5.7339e-04 (atm-liter³)/mol

b = -1.9727e-07 liter²

c = -5.521e-15 (atm-K²-liter³)/mol

α = -7.2673e-06 liter³

γ = 7.7942e-04 liter²

22.8 Results

At a gas temperature of 115°F (319 K), the required initial helium gas bottle should read, at a minimum, 1540 psig.

22.9 Conclusions

The initial helium gas bottle pressure was derived for the helium gas bottle at a temperature of 115°F. The initial required gas bottle pressure has been calculated to be 1540 psig. This calculation includes a minimum pressure of 200 psig is required to remain in the helium gas bottle after the 30 minute purge.

22.10 References

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Appendix A

PROBLEM 1

HELIUM INGRESS / Purge Cycle

1) Cask Void Space
 $V_1 = 0.53 \text{ ft}^3$

Ref: HNF-2933, Rev. 2

2) MCO Void Space
 $V_2 = 0.56 \text{ ft}^3$

Ref: HNF-2933, Rev. 2

- Assumptions:
- 1) Perfect mixing of gases between Cask and MCO void spaces
 - 2) H_2 generation constant at MCO water temperature (MCO water at constant temperature)
 - 3) Pressure quickly equalizes in the Cask and MCO void spaces (i.e. $P_{\text{MCO}} = P_{\text{Cask}}$)

Overall Balance

1) Cask Void Space

in: $\dot{n}_{\text{He}}$

out: $\dot{n}_i$

Accum: $\frac{dn_1}{dt}$

$$\frac{dn_1}{dt} = \dot{n}_{\text{He}} - \dot{n}_i$$

$$\frac{dn_1}{dt} = \dot{n}_{\text{He}} - \left(\frac{dn_2}{dt} - \dot{n}_{\text{H}_2} \right)$$

2) MCO Void Space

in: $\dot{n}_i + \dot{n}_{\text{H}_2}$

out: 0

Accum: $\frac{dn_2}{dt}$

$$\frac{dn_2}{dt} = \dot{n}_i + \dot{n}_{\text{H}_2}$$

$$\dot{n}_i = \frac{dn_2}{dt} - \dot{n}_{\text{H}_2}$$

$$\frac{dn_1}{dt} = \dot{n}_{He} - \left(\frac{dn_2}{dt} - \dot{n}_{He} \right)$$

or

$$\frac{dn_1}{dt} = \dot{n}_{He} + \dot{n}_{He} - \frac{dn_2}{dt}$$

Since pressure quickly equalizes in both MCO and Cask,

$$n_1 V_2 = n_2 V_1$$

$$P = \frac{n_1 R T}{V_1} = \frac{n_2 R T}{V_2}$$

and change in g/mol per time
at constant V_i

or $\frac{n_1}{V_1} = \frac{n_2}{V_2}$

$$V_2 \frac{dn_1}{dt} = V_1 \frac{dn_2}{dt}$$

or $\frac{dn_1}{dt} = \frac{V_1}{V_2} \frac{dn_2}{dt}$

let $k = \frac{V_1}{V_2}$

from above eqn,

$$\therefore k \frac{dn_2}{dt} = \dot{n}_{He} + \dot{n}_{He} - \frac{dn_2}{dt}$$

$$(k+1) \frac{dn_2}{dt} = \dot{n}_{He} + \dot{n}_{He}$$

$$dn_2 = \frac{(\dot{n}_{He} + \dot{n}_{He}) dt}{(k+1)}$$

let $\alpha = \frac{(\dot{n}_{He} + \dot{n}_{He})}{(k+1)}$

integrating,

$$n_2 = \alpha t + n_2^0$$

at $t=0$ $n_1 = n_1^0$
 $n_2 = n_2^0$

and since

$$n_2 = \frac{V_2}{V_1} n_1$$

$$n_2^0 = \frac{V_2}{V_1} n_1^0$$

$$n_1 = k \alpha t + n_1^0$$

Therefore,

$$n_1 = k\alpha t + n_1^0$$

$$n_2 = \alpha t + n_2^0$$

$$\dot{n}_1 = \frac{dn_1}{dt} - \dot{n}_{H_2}$$

$$= \alpha - \dot{n}_{H_2}$$

$$k = V_1/V_2$$

$$\alpha = \frac{(\dot{n}_{H_2} + \dot{n}_{H_2})}{(k+1)}$$

Hydrogen (H_2) Balance during Purge Cycle

y_1 : gmol H_2 fraction in Cask

y_2 : gmol H_2 fraction in MCO

1) Cask Void Space

in: 0

out: $y_1 \dot{n}_1$

Accum: $\frac{d(y_1 n_1)}{dt}$

2) MCO Void Space

in: $y_1 \dot{n}_1 + \dot{n}_{H_2}$

out: 0

Accum: $\frac{d(y_2 n_2)}{dt}$

Solving y_1 Around Cask

$$\frac{d(y_1 n_1)}{dt} = 0 - \dot{n}_1 y_1$$

$$\dot{n}_1 = \alpha - \dot{n}_{H_2}$$

$$n_1 \frac{dy_1}{dt} + y_1 \frac{dn_1}{dt} = -\dot{n}_1 y_1 = -(\alpha - \dot{n}_{H_2}) y_1$$

$$n_1 \frac{dy_1}{dt} + k\alpha y_1 + (\alpha - \dot{n}_{H_2}) y_1 = 0$$

$$n_1 \frac{dy_1}{dt} + k\alpha y_1 + \alpha y_1 - \dot{n}_{H_2} y_1 = 0 \quad A-4$$

$$\eta_1 \frac{dy_1}{dt} + [\alpha(k+1) - \dot{n}_{n2}] y_1 = 0$$

Can solve this ode if "exact", in other words put into form,

$$N(t, y_1) \frac{dy_1}{dt} + M(t, y_1) = 0$$

and to be "exact" $\frac{dN(t, y_1)}{dt} = \frac{d(M(t, y_1))}{dy_1}$

checking for "exactness",

$$\eta_1 = kt + \eta_0$$

$$\frac{dM}{dy_1} = \alpha(k+1) - \dot{n}_{n2} \quad \frac{dN}{dt} = k\alpha \quad \text{not exact!}$$

Not exact, therefore need an integration factor μ

such that: $\frac{d(\mu M)}{dy_1} = \frac{d(\mu N)}{dt}$

$$\mu \frac{dM}{dy_1} + M \frac{d\mu}{dy_1} = \mu \frac{dN}{dt} + N \frac{d\mu}{dt}$$

Breun 1983)

$$\therefore \frac{d\mu}{dt} = \left[\frac{\frac{dM}{dy_1} - \frac{dN}{dt}}{N} \right] \mu$$

Solving for μ ,

$$\frac{d\mu}{dt} = \left[\frac{(\alpha(k+1) - \dot{n}_{n2} - k\alpha)}{kt + \eta_0} \right] \mu = \left(\frac{\alpha - \dot{n}_{n2}}{kt + \eta_0} \right) \mu$$

$$\frac{d\mu}{\mu} = \left(\frac{\alpha - \dot{n}_{n2}}{kt + \eta_0} \right) dt$$

$$\ln \mu = \frac{(\alpha - \dot{n}_{n2})}{k\alpha} \ln(kt + \eta_0)$$

$$\text{let } \gamma = \frac{\alpha - \dot{n}_{n2}}{k\alpha}$$

$$\mu = \eta_1^\gamma$$

Now multiplying all terms by the integration factor,

$$\underbrace{\eta_1^\delta \eta_1}_{N^I} \frac{dy_1}{dt} + \underbrace{\eta_1^\delta [\alpha(k+1) - \dot{n}_{H_2}]}_{M^I} y_1 = 0$$

Therefore, checking "exactness"

$$\frac{\partial M^I}{\partial y_1} = \eta_1^\delta [\alpha(k+1) - \dot{n}_{H_2}] -$$

$$\delta + 1 = \frac{\alpha - \dot{n}_{H_2} + k\alpha}{k\alpha}$$

$$\frac{\partial N^I}{\partial t} = (\delta + 1) \eta_1^\delta (k\alpha)$$

$$= (\alpha(k+1) - \dot{n}_{H_2}) \eta_1^\delta -$$

Exact, therefore, there exists a function Ψ such that

$$\frac{\partial \Psi}{\partial y_1} \frac{dy_1}{dt} + \frac{\partial \Psi}{\partial t} = 0$$

where, $\frac{\partial \Psi}{\partial t} = M^I = \eta_1^\delta [\alpha(k+1) - \dot{n}_{H_2}] y_1$

General Sol'n: $\Psi = \alpha k [\alpha(k+1) - \dot{n}_{H_2}] (\delta + 1) y_1 \eta_1^{\delta+1} + h(y_1) = C$

$$= \alpha k [\alpha(k+1) - \dot{n}_{H_2}] \left[\frac{\alpha(k+1) - \dot{n}_{H_2}}{k\alpha} \right] y_1 \eta_1^{\delta+1} + h(y_1)$$

$$\rightarrow = [\alpha(k+1) - \dot{n}_{H_2}]^2 y_1 \eta_1^{\delta+1} + h(y_1) = C$$

and

$$\frac{\partial \Psi}{\partial y_1} = [\alpha(k+1) - \dot{n}_{H_2}]^2 \eta_1^{\delta+1} + h'(y_1)$$

Setting this equal to $\frac{\partial \Psi}{\partial y_1} = \eta_1^{\delta+1}$

$$\therefore h'(y_1) = \eta_1^{\delta+1} (1 - [\alpha(k+1) - \dot{n}_{H_2}])$$

and

$$h(y_1) = \eta_1^{\delta+1} (1 - [\alpha(k+1) - \dot{n}_{H_2}]) y_1$$

Now substituting into the general solution:

$$[\alpha(k+1) - \dot{n}_m]^2 y_1 \eta_1^{\delta+1} + (1 - [\alpha(k+1) - \dot{n}_m]) y_1 \eta_1^{\delta+1} = C$$

at initial conditions,

$$t=0$$

$$y_1 = y_1^0$$

$$\eta_1 = \eta_1^0$$

Simplifying,

$$\text{let } \beta = \alpha(k+1) - \dot{n}_m$$

$$\therefore \beta^2 y_1 (k\Delta t + \eta_1^0)^{\delta+1} + (1-\beta) y_1 (k\Delta t + \eta_1^0)^{\delta+1} = C$$

$$(k\Delta t + \eta_1^0)^{\delta+1} (\beta^2 - \beta + 1) y_1 = C$$

$$C = \eta_1^0{}^{\delta+1} (\beta^2 - \beta + 1) y_1^0$$

and substituting into general solution,

$$\eta_1^{\delta+1} (\beta^2 - \beta + 1) y_1 = \eta_1^0{}^{\delta+1} (\beta^2 - \beta + 1) y_1^0$$

$$\therefore y_1 = \frac{\eta_1^0{}^{\delta+1}}{\eta_1^{\delta+1}} y_1^0 = \frac{\eta_1^0{}^{\delta+1}}{(k\Delta t + \eta_1^0)^{\delta+1}} y_1^0$$

want to find $y_1 = f(P)$

$$\text{note: } \eta_1^0 = \frac{P^0 V_1}{RT} \quad \text{or} \quad P^0 = \eta_1^0 \frac{RT}{V_1}$$

$$\eta_1 = \frac{PV_1}{RT} = k\Delta t + \eta_1^0$$

Solving for P:

$$P = \frac{RT}{V_1} (k\Delta t + \eta_1^0)$$

taking ratio,

$$\frac{P}{P^0} = \frac{RT/V_1 (kdt + \eta_1^0)}{RT/V_1 \eta_1^0} = \frac{(kdt + \eta_1^0)}{\eta_1^0} = \frac{kdt}{\eta_1^0} + 1$$

or

$$kdt = \frac{P_{\eta_1^0}}{P^0} - \eta_1^0$$

now substituting into $y_1 = \frac{\eta_1^0}{(kdt + \eta_1^0)^{\delta+1}} y_1^0$

$$y_1 = \frac{\eta_1^0}{\left(\frac{P_{\eta_1^0}}{P^0}\right)^{\delta+1}} y_1^0 = \left(\frac{P^0}{P}\right)^{\delta+1} y_1^0 \quad \leftarrow \text{soln to } y_1 \text{ (check)}$$

Hydrogen Balance Around MCO

$$\frac{d(y_2 \eta_2)}{dt} = y_1 \dot{n}_1 + \dot{n}_{H_2}$$

$$\dot{n}_1 = \alpha - \dot{n}_{H_2}$$

$$\eta_2 = \alpha t + \eta_2^0$$

$$\eta_2 \frac{dy_2}{dt} + y_2 \frac{d\eta_2}{dt} = (\alpha - \dot{n}_{H_2}) y_1 + \dot{n}_{H_2}$$

$$\eta_2 \frac{dy_2}{dt} + \alpha y_2 - (\alpha - \dot{n}_{H_2}) y_1 - \dot{n}_{H_2} = 0$$

$$\eta_2 \frac{dy_2}{dt} + \alpha y_2 + \dot{n}_{H_2} y_1 - \alpha y_1 - \dot{n}_{H_2} = 0$$

$$\eta_2 \frac{dy_2}{dt} + \alpha y_2 + (\dot{n}_{H_2} - \alpha) y_1 - \dot{n}_{H_2} = 0$$

substituting in $y_1 = \frac{\eta_1^0}{\eta_1^{\delta+1}} y_1^0$ into the above eqn

$$n_2 \frac{dy_2}{dt} + \alpha y_2 + (\dot{n}_{H_2} - \alpha) \frac{n_1^{0+\delta+1}}{n_1^{0+\delta}} y_1^0 - \dot{n}_{H_2} = 0$$

$$n_1 = k\alpha t + n_1^0$$

$$n_2 = \alpha t + n_2^0$$

and checking for "exactness"

$$\frac{\partial M}{\partial y_2} = \alpha \quad \frac{\partial N}{\partial t} = \alpha \quad \text{exact} \quad \frac{\partial M}{\partial y_2} = \frac{\partial N}{\partial t}$$

Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = \alpha y_2 + (\dot{n}_{H_2} - \alpha) \frac{n_1^{0+\delta+1}}{n_1^{0+\delta}} y_1^0 - \dot{n}_{H_2}$$

note:

$$\int (a+bx)^n dx = \frac{(a+bx)^{n+1}}{(n+1)b}$$

$$\text{let } n = -(\delta+1) = -\delta - 1$$

$$\text{then } n+1 = -\delta$$

$$\psi = \alpha y_2 t - \dot{n}_{H_2} t + (\dot{n}_{H_2} - \alpha) \frac{n_1^{0+\delta+1}}{n_1^{0+\delta}} y_1^0 \left[\frac{n_1^{-\delta}}{(-\delta)(k\alpha)} \right] + h(y_2) = C$$

$$n_1 = k\alpha t + n_1^0$$

$$(-\delta)(k\alpha):$$

$$\delta = \frac{\alpha - \dot{n}_{H_2}}{k\alpha}$$

$$\delta(k\alpha) = \alpha - \dot{n}_{H_2}$$

$$-\delta(k\alpha) = (\dot{n}_{H_2} - \alpha)$$

$$\psi = \alpha y_2 t - \dot{n}_{H_2} t + y_1^0 \frac{n_1^{0+\delta+1}}{n_1^{0+\delta}} + h(y_2) = C$$

then

$$\frac{\partial \psi}{\partial y_2} = \alpha t + h'(y_2)$$

$$\text{Setting equal to } \frac{\partial \psi}{\partial y_2} = n_2 = \alpha t + n_2^0 = \alpha t + h'(y_2)$$

$$\therefore h'(y_2) = n_2^0 \quad \text{and} \quad \therefore h(y_2) = n_2^0 y_2$$

Substituting into general equation:

$$\alpha y_2 t - \dot{n}_{H_2} t + y_1^0 \frac{n_1^{0+\delta+1}}{n_1^{0+\delta}} + n_2^0 y_2 = C$$

Solving for C, @ initial conditions, $t=0$

$$C = y_1^0 \frac{n_1^{0\delta+1}}{n_1^{0\delta}} + n_2^0 y_2^0 = y_1^0 n_1^0 + y_2^0 n_2^0$$

$y_2 = y_2^0$
 $n_1 = n_1^0$

and substituting into general eqn:

$$\alpha y_2 t - \dot{n}_2 t + y_1^0 \frac{n_1^{0\delta+1}}{n_1^{0\delta}} + n_2^0 y_2 = y_1^0 n_1^0 + y_2^0 n_2^0$$

and solving for y_2 ,

$$y_2 (\alpha t + n_2^0) = y_1^0 n_1^0 + y_2^0 n_2^0 + \dot{n}_2 t - y_1^0 \frac{n_1^{0\delta+1}}{n_1^{0\delta}}$$

$$n_2 y_2 = y_1^0 n_1^0 \left(1 - \frac{n_1^{0\delta}}{n_1^{0\delta+1}}\right) + y_2^0 n_2^0 + \dot{n}_2 t$$

$$y_2 = \frac{y_1^0 n_1^0}{n_2} \left(1 - \frac{n_1^{0\delta}}{n_1^{0\delta+1}}\right) + y_2^0 \frac{n_2^0}{n_2} + \frac{\dot{n}_2 t}{n_2}$$

from previous equalities:

$$\frac{n_2^0}{n_2} = \frac{P^0}{P} = \frac{n_1^0}{n_1}$$

putting in terms of P,

and

$$n_2 = \alpha t + n_2^0 = n_2^0 \frac{P}{P^0}$$

$$y_2 = y_1^0 \left(\frac{P^0}{P} \right) \left[1 - \left(\frac{P^0}{P} \right)^{\delta} \right] + y_2^0 \left(\frac{P^0}{P} \right) + \frac{\dot{n}_2}{\alpha} \left(1 - \frac{P^0}{P} \right)$$

$$n_1^0 = \frac{P^0 V_1}{RT}$$

$$n_2 = \frac{P V_2}{RT}$$

$$\frac{n_1^0}{n_2} = \frac{P^0 V_1 / RT}{P V_2 / RT} = \frac{P^0}{P} \frac{V_1}{V_2} = \frac{P^0}{P} k$$

$$n_2 = \alpha t + n_2^0$$

$$\frac{n_2}{n_2^0} = \frac{\alpha t}{n_2^0} + \frac{n_2^0}{n_2^0}$$

$$\frac{1}{\alpha} = \frac{t}{n_2} + \frac{n_2^0}{\alpha n_2}$$

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$$\frac{t}{n_2} = \frac{1}{\alpha} - \frac{n_2^0}{\alpha n_2} = \frac{1}{\alpha} \left(1 - \frac{n_2^0}{n_2} \right) = \frac{1}{\alpha} \left(1 - \frac{P^0}{P} \right)$$

Therefore, exact solutions for Purge Cycle:

$$y_1 = \left(\frac{P^0}{P}\right)^{\delta+1} y_1^0$$

$$\delta = \frac{d - \dot{n}_{u2}}{k d}$$

$$d = \frac{(\dot{n}_{u2} + \dot{n}_{m2})}{(k+1)}$$

$$k = \frac{V_1}{V_2}$$

$$y_2 = y_1^0 k \frac{P^0}{P} \left[1 - \left(\frac{P^0}{P}\right)^{\delta} \right] + y_2^0 \left(\frac{P^0}{P}\right) + \frac{\dot{n}_{u2}}{d} \left(1 - \frac{P^0}{P} \right)$$

Bleed Cycle

1) Cask Void Space

2) MCO Void Space

Overall Balance

Cask Space

in: $\dot{n}_i$

out: $\dot{n}_{ex}$

Accum: $\frac{dn_1}{dt}$

$$\frac{dn_1}{dt} = \dot{n}_i - \dot{n}_{ex}$$

$$\frac{dn_1}{dt} = \left(\dot{n}_{H_2} - \frac{dn_2}{dt} \right) - \dot{n}_{ex}$$

MCO Space

in: $\dot{n}_{H_2}$

out: $\dot{n}_i$

Accum: $\frac{dn_2}{dt}$

$$\frac{dn_2}{dt} = \dot{n}_{H_2} - \dot{n}_i$$

$$\dot{n}_i = \dot{n}_{H_2} - \frac{dn_2}{dt}$$

$$\text{since } \frac{dn_1}{dt} = \frac{V_1}{V_2} \frac{dn_2}{dt} = k \frac{dn_2}{dt}$$

$$k \frac{dn_2}{dt} = \dot{n}_{H_2} - \frac{dn_2}{dt} - \dot{n}_{ex}$$

$$(k+1) \frac{dn_2}{dt} = \dot{n}_{H_2} - \dot{n}_{ex}$$

$$\frac{dn_2}{dt} = \frac{(\dot{n}_{H_2} - \dot{n}_{ex})}{(k+1)} = \beta$$

$$\text{let } \beta = \frac{(\dot{n}_{H_2} - \dot{n}_{ex})}{(k+1)}$$

$$\frac{dn_2}{dt} = \beta$$

$$n_2 - n_2^0 = \beta t$$

$$n_2 = \beta t + n_2^0$$

$$\text{Since } n_2 = \frac{v_2}{v_1} n_1$$

$$n_2^0 = \frac{v_2}{v_1} n_1^0$$

$$\frac{v_2}{v_1} n_1 = \beta t + \frac{v_2}{v_1} n_1^0$$

$$\therefore n_1 = k\beta t + n_1^0$$

$$n_1 = k\beta t + n_1^0$$

$$n_2 = \beta t + n_2^0$$

$$n_i = \dot{n}_{H_2} - \beta$$

$$k = v_1/v_2$$

$$\beta = \frac{(\dot{n}_{H_2} - \dot{n}_{ex})}{(k+1)}$$

Hydrogen Balance Around Cask

$$\text{in: } y_2 \dot{n}_i$$

$$\text{out: } y_1 \dot{n}_{ex}$$

$$\text{Accum: } \frac{d(n, y_1)}{dt}$$

$$\frac{d(n, y_1)}{dt} = \dot{n}_i y_2 - \dot{n}_{ex} y_1$$

$$n_1 \frac{dy_1}{dt} + y_1 \frac{dn_1}{dt} = (\dot{n}_{H_2} - \beta) y_2 - \dot{n}_{ex} y_1$$

$$n_1 \frac{dy_1}{dt} + k\beta y_1 = (\dot{n}_{H_2} - \beta) y_2 + \dot{n}_{ex} y_1 = 0$$

$$n_1 \frac{dy_1}{dt} + (k\beta + \dot{n}_{ex}) y_1 - (\dot{n}_{H_2} - \beta) y_2 = 0$$

need to solve numerically,

Therefore, set up for RK solver (as in Purge Cycle around the MCO). Since substitution of y_2 into this eqn results in an "ugly" integration.

$$\eta_1 \frac{dy_1}{dt} = (\dot{n}_{H_2} - \beta) y_2 - (k\beta + \dot{n}_{Ex}) y_1$$

$$\frac{dy_1}{dt} = \frac{1}{\eta_1} [(\dot{n}_{H_2} - \beta) y_2 - (k\beta + \dot{n}_{Ex}) y_1]$$

$$\eta_1 = \frac{PV_1}{RT}$$

$$\frac{dy_1}{dt} = \frac{RT}{PV_1} [(\dot{n}_{H_2} - \beta) y_2 - (k\beta + \dot{n}_{Ex}) y_1]$$

Hydrogen Balance Around MCO

in: $\dot{n}_{H_2}$

out: $y_2 \dot{n}_i$

Accum: $\frac{d(n_2 y_2)}{dt}$

$$n_2 = \beta t + n_2^0$$

$$\eta_i = \dot{n}_{H_2} - \beta$$

$$\beta = \frac{(\dot{n}_{H_2} - \dot{n}_{Ex})}{(k+1)}$$

$$\frac{d(n_2 y_2)}{dt} = \dot{n}_{H_2} - y_2 \dot{n}_i$$

$$n_2 \frac{dy_2}{dt} + y_2 \frac{dn_2}{dt} = \dot{n}_{H_2} - y_2 (\dot{n}_{H_2} - \beta)$$

$$n_2 \frac{dy_2}{dt} + \beta y_2 + y_2 (\dot{n}_{H_2} - \beta) - \dot{n}_{H_2} = 0$$

$$n_2 \frac{dy_2}{dt} + \dot{n}_{H_2} y_2 - \dot{n}_{H_2} = 0$$

checking "exactness"

$$\frac{\partial M}{\partial y_2} = \dot{n}_{H_2} \quad \frac{\partial N}{\partial t} = \beta \quad \text{not exact}$$

therefore, need to solve for Integration Factor, μ

$$\frac{d\mu}{dt} = \left[\frac{\dot{n}_{H_2} - \beta}{n_2} \right] \mu$$

$$\int \frac{d\mu}{\mu} = (\dot{n}_{H_2} - \beta) \int \frac{1}{(\beta t + n_2^0)} dt$$

$$\ln \mu = \frac{(\dot{n}_{H_2} - \beta)}{\beta} \ln n_2 \quad \text{let } \phi = \frac{(\dot{n}_{H_2} - \beta)}{\beta}$$

$$\mu = n_2^\phi$$

Now multiplying all terms by μ ,

$$\underbrace{n_2^{\phi+1}}_{\mu} \frac{dy_2}{dt} + \underbrace{n_2^\phi \dot{n}_{H_2} (y_2 - 1)}_{\text{ms}} = 0$$

checking "exactness"

$$\frac{\partial M^\dagger}{\partial y_2} = n_2^\phi \dot{n}_{H_2} - \frac{\partial N^\dagger}{\partial t} = (\phi+1) n_2^\phi \beta$$

Therefore, there exists ψ such that

$$\rho(\phi+1) = \frac{\dot{n}_{H_2} \cdot \beta}{\beta} = \frac{\text{exact}}{n_{H_2}}$$

$$\frac{\partial \psi}{\partial t} = n_2^\phi \dot{n}_{H_2} (y_2 - 1)$$

$$\psi = \frac{\dot{n}_{H_2} (y_2 - 1) n_2^{\phi+1}}{(\phi+1)\beta} + h(y_2) = C$$

and

$$\frac{\partial \psi}{\partial y_2} = n_2^{\phi+1} \neq h'(y_2)$$

Therefore, setting equal to $\frac{\partial \psi}{\partial y_2} = N^I = n_2^{\phi+1}$

$$h'(y_2) = 0 \quad \text{and} \quad h(y_2) = 0$$

Substituting into general equation,

$$(y_2 - 1) n_2^{\phi+1} = C$$

Solve for C @ initial conditions

$$\tau = 0$$

$$y_2 = y_2^0$$

$$(y_2^0 - 1) n_2^{\phi+1} = C$$

and substituting into eqn,

$$(y_2 - 1) n_2^{\phi+1} = (y_2^0 - 1) n_2^{\phi+1}$$

and solving for y_2 ,

$$y_2 - 1 = \frac{n_2^{\phi+1}}{n_2^{\phi+1}} (y_2^0 - 1)$$

$$y_2 = \frac{n_2^{\phi+1}}{n_2^{\phi+1}} (y_2^0 - 1) + 1 = \frac{n_2^{\phi+1}}{(\beta t + n_2^0)^{\phi+1}} (y_2^0 - 1) + 1$$

in terms of P ,
as before, $n_2^0 = \frac{P^0 V_2}{RT}$

$$\frac{P}{P^0} = \frac{\frac{RT}{V_2} (\beta t + n_2^0)}{RT n_2^0}$$

$$\therefore \beta t = n_2^0 \frac{P}{P^0} - n_2^0$$

$$n_2 = \frac{P V_2}{RT} = \beta t + n_2^0$$

$$P = \frac{RT}{V_2} (\beta t + n_2^0)$$

$$P^0 = \frac{n_2^0 RT}{V_2}$$

Substituting into solution,

$$y_2 = \frac{\eta_2^{\phi+1}}{(\beta t + \eta_2^0)^{\phi+1}} (y_2^0 - 1) + 1 = \left(\frac{P^0}{P}\right)^{\phi+1} (y_2^0 - 1) + 1$$

Therefore, set up for RK solver as

$$y_2 = \left(\frac{P^0}{P}\right)^{\phi+1} (y_2^0 - 1) \quad \leftarrow \text{exact sol'n}$$

$$\phi+1 = \frac{\dot{n}_{H_2}}{\beta}$$

$$\beta = \frac{(\dot{n}_{H_2} - \dot{n}_{ex})}{(k+1)}$$

$$\frac{dy_1}{dt} = \frac{RT}{PV_1} \left[(\dot{n}_{H_2} - \beta) y_2 - (k\beta + \dot{n}_{ex}) y_1 \right]$$

$$k = V_1/V_2$$

Since the y_1 cannot be solved easily analytically, the Runge-Kutta method is used. The RK method integrates with respect to time, whereas in the exact solution, the time variable is substituted by a pressure term, i.e., $k\alpha t = \frac{P\eta_2^0}{P^0} - \eta_2^0$

from the overall mass balance. Therefore, the same correlation between pressure and time must be utilized in the RK routine, i.e. in integrating, for each pressure step taken, a correlated time step must be used as shown above.

integrate over
T/P range:

$$\text{i.e. } \frac{\Delta t}{\Delta P} = \frac{t_{\text{final}} - t_{\text{start}}}{P_{\text{final}} - P_{\text{start}}} = \frac{t_{\text{final}}}{20 \text{ psi}}$$

$$t_{\text{final}} = \frac{\eta_1^0}{k\alpha} \left(\frac{P}{P^0} - 1 \right) \quad \text{for } P = 15.2 \text{ to } 35.2$$

Perfect
Mixing

during Delay

Problem 1 - DELAY

①

MCOOverall BalanceCaskin: i_{H2} in: i_i out: i_i

out: 0

Accum: $\frac{dn_2}{dt}$ Accum: $\frac{dn_1}{dt}$

$$\frac{dn_2}{dt} = i_{H2} - i_i$$

$$\frac{dn_1}{dt} = i_i$$

$$P = \frac{n_1}{V_1} = \frac{n_2}{V_2} \quad k = \frac{V_1}{V_2}$$

$$\text{or } n_1 = k n_2$$

$$\frac{dn_1}{dt} = k \frac{dn_2}{dt}$$

$$\frac{dn_2}{dt} = i_{H2} - \frac{dn_1}{dt} = i_{H2} - k \frac{dn_2}{dt}$$

$$(k+1) \frac{dn_2}{dt} = i_{H2}$$

$$\frac{dn_2}{dt} = \frac{i_{H2}}{(k+1)} = \alpha'$$

$$n_2 - n_2^0 = \alpha' t$$

$$\therefore n_2 = \alpha' t + n_2^0 \quad \text{A-18}$$

$$\frac{dn_2}{dt} = \alpha'$$

$$i_i = \frac{dn_1}{dt} = k \frac{dn_2}{dt} = k \alpha'$$

H₂ BalanceMCOin: $\dot{n}_{H_2}$ out: $\dot{n}_2 y_2$ Accum: $\frac{d(n_2 y_2)}{dt}$

$$n_2 \frac{dy_2}{dt} + y_2 \frac{dn_2}{dt} = \dot{n}_{H_2} - \dot{n}_2 y_2 + k \frac{dn_2}{dt}$$

$$n_2 \frac{dy_2}{dt} + \frac{dn_2}{dt} (y_2 + k) - \dot{n}_{H_2} = 0$$

$$n_2 \frac{dy_2}{dt} + y_2 \alpha' + k \alpha' - \dot{n}_{H_2} = 0$$

checking "exactness"

$$\frac{\partial M}{\partial y_2} = \alpha' \quad \frac{\partial N}{\partial t} = \alpha' \quad \checkmark \quad \text{exact}$$

Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = y_2 \alpha' + k \alpha' - \dot{n}_{H_2}$$

General Soln

$$\therefore \psi = (y_2 \alpha' + k \alpha' - \dot{n}_{H_2}) t + h(y_2) = C$$

$$\therefore \frac{\partial \psi}{\partial y_2} = \alpha' t + h'(y_2)$$

$$\text{Setting equal to } \frac{\partial \psi}{\partial y_2} = \alpha' t + n_2^0$$

$$\therefore h'(y_2) = n_2^0 \quad \text{and} \quad h(y_2) = n_2^0 y_2$$

Substituting into General Solution:

$$(y_2 \alpha' + k \alpha' - \dot{n}_{H_2})t + n_2^0 y_2 = C$$

Solving for C, @ initial conditions, $t=0$
 $y_2 = y_2^0$

$$C = n_2^0 y_2^0$$

Therefore, sol'n is:

$$(y_2 \alpha' + k \alpha' - \dot{n}_{H_2})t + n_2 y_2 = n_2^0 y_2^0$$

and solving for y_2 :

$$y_2 \alpha' t + k \alpha' t - \dot{n}_{H_2} t + n_2 y_2 = n_2^0 y_2^0$$

$$y_2 (\alpha' t + n_2^0) = n_2^0 y_2^0 + \dot{n}_{H_2} t - k \alpha' t$$

$$y_2 = \frac{(\dot{n}_{H_2} - k \alpha')t}{(\alpha' t + n_2^0)} + \frac{n_2^0 y_2^0}{(\alpha' t + n_2^0)}$$

note: $n_2 = \alpha' t + n_2^0 = \frac{P V_2}{RT}$
 $n_2^0 = \frac{P^0 V_2}{RT}$

$$y_2 = \frac{RT(\dot{n}_{H_2} - k \alpha')t}{P V_2} + \frac{P^0}{P} y_2^0$$

or

$$y_2 = \frac{1}{P} \left[\frac{RT}{V_2} (\dot{n}_{H_2} - k \alpha')t + P^0 y_2^0 \right]$$

or

$$P = n \frac{RT}{V}$$

$$y_2 = \frac{1}{n_2} (\dot{n}_{H_2} - k \alpha')t + \frac{n_2^0}{n_2} y_2^0$$

note $n_2 = f(t)$ A-20 $n_2 = \alpha' t + n_2^0$

CZSK

H₂ Balancein: $\dot{n}_1 y_2$

$$\dot{n}_1 = \frac{dn_1}{dt}$$

out: 0

Accum: $\frac{d(n_1 y_1)}{dt}$

$$\dot{n}_1 \frac{dy_1}{dt} + y_1 \frac{dn_1}{dt} = y_2 \frac{dn_1}{dt}$$

$$\dot{n}_1 \frac{dy_1}{dt} + \frac{dn_1}{dt} [y_1 - y_2] = 0$$

$$\dot{n}_1 \frac{dy_1}{dt} + k_d' y_1 - k_d' y_2 = 0$$

$$y_2 = \frac{1}{\dot{n}_2} (\dot{n}_{H_2} - k_d') t + \frac{n_2^0}{\dot{n}_2} y_1^0$$

$$\frac{dn_1}{dt} = k_d'$$

$$n_1 = k_d' t + n_1^0$$

checking "exactness":

$$\frac{\partial M}{\partial y_1} = k_d' \quad \frac{\partial N}{\partial t} = k_d' \quad \text{exact}$$

Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = k_d' y_1 - k_d' \left[\frac{1}{\dot{n}_2} (\dot{n}_{H_2} - k_d') t + \frac{n_2^0}{\dot{n}_2} y_1^0 \right]$$

$$\frac{\partial \psi}{\partial t} = k_d' y_1 - k_d' \left[\frac{(\dot{n}_{H_2} - k_d') t}{(\dot{n}_2 t + n_2^0)} + \frac{n_2^0 y_1^0}{(\dot{n}_2 t + n_2^0)} \right]$$

$$\frac{\partial \psi}{\partial t} = k_d' y_1 - \frac{k_d' (\dot{n}_{H_2} - k_d') t}{(\dot{n}_2 t + n_2^0)} - \frac{k_d' n_2^0 y_1^0}{(\dot{n}_2 t + n_2^0)}$$

$$\text{note: } \int \frac{t}{(a+bt)} dt = \frac{t}{b} - \frac{a}{b^2} \ln|a+bt|$$

$$\text{and } \int \frac{1}{(a+bt)} dt = \frac{1}{b} \ln|a+bt|$$

General Sol'n
→

$$\begin{aligned} \text{let } A &= kd' \\ B &= A(n_2^0 - kd') \\ C &= A n_2^0 y_2^0 \end{aligned}$$

$$\frac{\partial \psi}{\partial t} = A y_1 - \frac{B t}{(\alpha' t + n_2^0)} - \frac{C}{(\alpha' t + n_2^0)}$$

$$\psi = A y_1 t - B \left[\frac{t}{\alpha'} - \frac{n_2^0}{\alpha'^2} \ln n_2 \right] - \frac{C}{\alpha'} \ln n_2 + h(y_1) = C'$$

and

$$\frac{\partial \psi}{\partial y_1} = A t + h'(y_1) \text{ or } kd' t + h'(y_1)$$

$$\text{setting equal to } \frac{\partial \psi}{\partial y_1} = kd' t + n_1^0$$

$$\therefore h'(y_1) = n_1^0 \text{ and } h(y_1) = n_1^0 y_1$$

substituting into general sol'n:

$$A y_1 t - \frac{B t}{\alpha'} + \frac{B n_2^0}{\alpha'^2} \ln n_2 - \frac{C}{\alpha'} \ln n_2 + n_1^0 y_1 = C'$$

Solving for C' @ initial conditions, $t=0$
 $y_1 = y_1^0$

$$C' = \frac{B n_2^0}{\alpha'^2} \ln n_2^0 - \frac{C}{\alpha'} \ln n_2^0 + n_1^0 y_1^0$$

and substituting into general sol'n

$$A y_1 t - \frac{B t}{\alpha'} + \frac{B n_2^0}{\alpha'^2} \ln n_2 - \frac{C}{\alpha'} \ln n_2 + n_1^0 y_1 = \frac{B n_2^0}{\alpha'^2} \ln n_2^0 - \frac{C}{\alpha'} \ln n_2^0 + n_1^0 y_1^0$$

now solving for y_1 :

$$y_1 \underbrace{(At + n_1^0)}_{\eta_1} = \frac{B n_2^0}{\alpha'^2} (\ln n_2^0 - \ln n_2) - \frac{C}{\alpha'} (\ln n_2^0 - \ln n_2) + \frac{Bt}{\alpha'} + n_1^0 y_1^0$$

$$y_1 = \frac{1}{\eta_1} \left[(\ln n_2^0 - \ln n_2) \left(\frac{B n_2^0}{\alpha'^2} - \frac{C}{\alpha'} \right) + \frac{Bt}{\alpha'} + n_1^0 y_1^0 \right]$$

$$y_1 = \frac{1}{\eta_1} \left[\ln \left(\frac{n_2^0}{n_2} \right) \left[\frac{B n_2^0}{\alpha'^2} - \frac{C}{\alpha'} \right] + \frac{Bt}{\alpha'} + n_1^0 y_1^0 \right]$$

where $\frac{B n_2^0}{\alpha'^2} = \frac{k \alpha' (\dot{n}_{H_2} - k \alpha') n_2^0}{\alpha'^2} = \frac{k (\dot{n}_{H_2} - k \alpha') n_2^0}{\alpha'} = k n_1$

$$\frac{C}{\alpha'} = \frac{k \alpha' n_2^0 y_2^0}{\alpha'} = k n_2^0 y_2^0$$

$$\frac{Bt}{\alpha'} = \frac{k \alpha' (\dot{n}_{H_2} - k \alpha') t}{\alpha'} = \frac{k (\dot{n}_{H_2} - k \alpha') t}{\alpha'} = k \alpha' t$$

$$y_1 = \frac{1}{\eta_1} \left[\ln \left(\frac{n_2^0}{n_2} \right) (k n_2^0 - n_2^0 y_2^0) + k \alpha' t + n_1^0 y_1^0 \right]$$

$$y_1 = \ln \left(\frac{n_2^0}{n_2} \right) \left[k \frac{n_2^0}{\eta_1} - \frac{n_2^0}{\eta_1} y_2^0 \right] + \frac{k \alpha' t}{\eta_1} + \frac{n_1^0}{\eta_1} y_1^0$$

note: $k \alpha' t + n_1^0 = \eta_1$

or $k \alpha' t = \eta_1 - n_1^0$

$$\frac{n_1 - n_2^0}{\eta_1} = 1 - \frac{P^0}{P}$$

$$y_1 = \ln \left(\frac{P^0}{P} \right) \left(\frac{P^0}{P} - \frac{P^0}{k P} y_2^0 \right) + 1 - \frac{P^0}{P} + \frac{P^0}{P} y_1^0$$

$$y_1 = \ln \left(\frac{P^0}{P} \right) \left[1 - y_2^0 \right] \frac{P^0}{P} - \frac{P^0}{P} (1 - y_1^0) + 1$$

Appendix B

Problem 2 - high nominal H_2

11

- bounding H_2 $\dot{V}_2$ rate (gmol/min)

sh nominal: 0.0192

undings: $(2.4 \times 10^3 \text{ g/sec})$
0.072 gmol/min Purge CycleOverall Balancein: $\dot{n}_{He} + \dot{n}_{H_2}$

out: 0

$$\text{Accum: } \frac{dn_i}{dt} = \dot{n}_{He} + \dot{n}_{H_2}$$

at $t=0$

$$n = n^0$$

Hydrogen Balancein: $\dot{n}_{H_2}$

out: 0

$$\text{Accum: } \frac{d(ny)}{dt} = \dot{n}_{H_2}$$

$$n \frac{dy}{dt} + y \frac{dn_i}{dt} = \dot{n}_{H_2}$$

$$n \frac{dy}{dt} + y(\dot{n}_{He} + \dot{n}_{H_2}) = \dot{n}_{H_2}$$

$$n \frac{dy}{dt} + y(\dot{n}_{He} + \dot{n}_{H_2}) - \dot{n}_{H_2} = 0$$

$$n \frac{dy}{dt} + dy - \dot{n}_{H_2} = 0$$

$$\text{where } \frac{dn_i}{dt} = \dot{n}_{He} + \dot{n}_{H_2}$$

$$\int dn = \int (\dot{n}_{He} + \dot{n}_{H_2}) dt$$

$$n - n^0 = (\dot{n}_{He} + \dot{n}_{H_2}) t$$

$$n = (\dot{n}_{He} + \dot{n}_{H_2}) t + n^0$$

$$\text{let } \alpha = (\dot{n}_{He} + \dot{n}_{H_2})$$

$$n = \alpha t + n^0$$

checking for "exactness":

$$\text{let } M = \alpha y - \dot{n}_{H_2}$$

$$\therefore \frac{\partial M}{\partial y} = \alpha$$

$$\frac{\partial N}{\partial t} = \alpha \quad \text{exact}$$

$$N = n = \alpha t + n_0$$

exact, therefore,

There exists a ψ such that,

$$M = \frac{\partial \psi}{\partial t} = \alpha y - \dot{n}_{H_2}$$

$$\partial \psi = (\alpha y - \dot{n}_{H_2}) \partial t$$

$$\psi = (\alpha y - \dot{n}_{H_2}) t + h(y) = c$$

and then taking derivative w/respect to y ,

$$\frac{\partial \psi}{\partial y} = \alpha t + h'(y)$$

then setting this eqn to $\frac{\partial \psi}{\partial y} = N = \alpha t + n_0$

and solving for $h'(y)$ and $h(y)$:

$$\alpha t + h'(y) = \alpha t + n_0$$

$$\therefore h'(y) = n_0 \quad \text{and} \quad h(y) = n_0 y$$

Therefore, general equation:

$$\psi = (\alpha y - \dot{n}_{H_2}) t + n_0 y = c$$

then solve for c @ initial conditions,

$$\therefore c = n_0 y_0$$

$$t=0 \\ y=y_0$$

Therefore,

$$(\alpha y - \dot{n}_{H_2})t + n^{\circ}y - n^{\circ}y^{\circ} = 0$$

and solving for y :

$$n^{\circ}y = n^{\circ}y^{\circ} - (\alpha y - \dot{n}_{H_2})t = n^{\circ}y^{\circ} - \alpha y t + \dot{n}_{H_2}t$$

or

$$n^{\circ}y + \alpha y t = n^{\circ}y^{\circ} + \dot{n}_{H_2}t$$

and

$$y(n^{\circ} + \alpha t) = \dot{n}_{H_2}t + n^{\circ}y^{\circ}$$

$$\therefore y = \frac{\dot{n}_{H_2}t + n^{\circ}y^{\circ}}{(\alpha t + n^{\circ})}$$

$$\alpha t = \frac{n^{\circ}P}{P^{\circ}} - n^{\circ}$$

$$y = \frac{\dot{n}_{H_2}t + n^{\circ}y^{\circ}}{\left(\frac{n^{\circ}P}{P^{\circ}}\right)} = \frac{P^{\circ}}{n^{\circ}P} [\dot{n}_{H_2}t + n^{\circ}y^{\circ}]$$

$$y = \left(\frac{P^{\circ}}{P} \frac{\dot{n}_{H_2}}{n^{\circ}}\right)t + \frac{P^{\circ}}{P} y^{\circ}$$

and

$$t = \frac{n^{\circ}P}{\alpha P^{\circ}} - \frac{n^{\circ}}{\alpha}$$

$$y = \left(\frac{P^{\circ}}{P} \frac{\dot{n}_{H_2}}{n^{\circ}}\right) \left(\frac{P^{\circ}}{\alpha} a\right) + \frac{P^{\circ}}{P} y^{\circ}$$

$$= \frac{n^{\circ}}{\alpha} \underbrace{\left(\frac{P}{P^{\circ}} - 1\right)}_a$$

$$y = \frac{\dot{n}_{H_2}}{\alpha} \frac{P^{\circ}}{P} \left(\frac{P}{P^{\circ}} - 1\right) + \frac{P^{\circ}}{P} y^{\circ}$$

$$= \frac{a n^{\circ}}{\alpha}$$

$$y = \frac{\dot{n}_{H_2}}{\alpha} - \frac{\dot{n}_{H_2} P^{\circ}}{\alpha P} + \frac{P^{\circ}}{P} y^{\circ}$$

B-4

$$y = \frac{P^{\circ}}{P} (y^{\circ} - \frac{\dot{n}_{H_2}}{P^{\circ}}) + \frac{\dot{n}_{H_2}}{P}$$

$$n = \frac{PV}{RT} = \Delta t + n^0 = \Delta t + \frac{P^0 V}{RT}$$

$$n^0 = \frac{P^0 V}{RT}$$

$$\frac{P}{P^0} = \frac{\frac{RT}{V} (\Delta t + n^0)}{\frac{RT}{V} n^0}$$

$$\frac{P}{P^0} = \frac{\cancel{RT/V} (\Delta t + n^0)}{n^0 \cancel{RT/V}}$$

$$\therefore \frac{n^0 P}{P^0} = (\Delta t + n^0)$$

$$\Delta t = \frac{n^0 P}{P^0} - n^0$$

$$y = \frac{n^0}{(\beta t + n^0)^{\delta+1}} (y^0 - 1) + 1$$

where $\beta t = \frac{n^0 P}{P^0} - n^0$

$$\therefore y = \left(\frac{P^0}{P} \right)^{\delta+1} (y^0 - 1) + 1$$

$$\delta = \frac{\dot{n}_{ex}}{\beta} = \frac{\dot{n}_{ex}}{\dot{n}_{in} - \dot{n}_{ex}}$$

$$\beta = \dot{n}_{in} - \dot{n}_{ex}$$

$$\begin{aligned} \delta + 1 &= \frac{\dot{n}_{ex}}{(\dot{n}_{in} - \dot{n}_{ex})} + \frac{(\dot{n}_{in} - \dot{n}_{ex})}{(\dot{n}_{in} - \dot{n}_{ex})} \\ &= \frac{\dot{n}_{in}}{(\dot{n}_{in} - \dot{n}_{ex})} \end{aligned}$$

Vent CycleProblem 2 - high nominal n_2

11

Overall Balancein: $\dot{n}_{H_2}$ out: $\dot{n}_{EX}$

Accum: $\frac{dn}{dt} = \dot{n}_{H_2} - \dot{n}_{EX}$

C $t=0$
 $n = n^0$

$$\int dn = (\dot{n}_{H_2} - \dot{n}_{EX}) dt$$

$$\beta = \dot{n}_{H_2} - \dot{n}_{EX}$$

$$n - n^0 = \beta t$$

$$\therefore n = \beta t + n^0$$

Hydrogen Balancein: $\dot{n}_{H_2}$ out: $\dot{n}_{EX} y$

Accum: $\frac{d(ny)}{dt} = \dot{n}_{H_2} - \dot{n}_{EX} y$

$$n \frac{dy}{dt} + y \frac{dn}{dt} \stackrel{\beta}{=} \dot{n}_{H_2} - \dot{n}_{EX} y$$

$$n \frac{dy}{dt} + \underbrace{(\beta y + \dot{n}_{EX} y)}_{y(\beta + \dot{n}_{EX})} - \dot{n}_{H_2} = 0$$

Where: $\beta + \dot{n}_{EX} = \dot{n}_{H_2}$

Therefore,

$$n \frac{dy}{dt} + \underbrace{\dot{n}_{H_2} y - \dot{n}_{H_2}}_M = 0$$

checking for "exactness"

$$\frac{\partial M}{\partial y} = \dot{n}_{H_2}$$

$$\frac{\partial N}{\partial t} = \beta = \dot{n}_{H_2} - \dot{n}_{EX}$$

not exact!

Not exact, therefore need Integration Constant, μ

$$\frac{d\mu}{dt} = \left[\frac{M_y - N_t}{n} \right] \mu = \frac{(\dot{n}_{H_2} - \beta)}{n} \mu = + \frac{\dot{n}_{EX}}{n} \mu$$

$$\int \frac{d\mu}{\mu} = \int \frac{\dot{n}_{EX}}{n} dt$$

$$\beta = \dot{n}_{H_2} - \dot{n}_{EX}$$

$$(\dot{n}_{H_2} - (\dot{n}_{H_2} - \dot{n}_{EX})) = +\dot{n}_{EX}$$

$$\ln \mu = \frac{\dot{n}_{EX}}{\beta} \ln(\beta t + n^0)$$

$$\mu = n^{\dot{n}_{EX}/\beta} = n^{\delta} \quad \text{let } \delta = \frac{\dot{n}_{EX}}{\beta}$$

Therefore, multiplying all terms by $n^{\dot{n}_{EX}/\beta}$ or n^{δ}

$$n^{\delta+1} \frac{dy}{dt} + \underbrace{n^{\delta} (\dot{n}_{H_2} y - \dot{n}_{H_2})}_M = 0$$

checking "exactness"

$$\frac{\partial M^I}{\partial y} = n^{\delta} (\dot{n}_{H_2})$$

$$\frac{\partial N^I}{\partial t} = (\delta+1) n^{\delta} \dot{n}_{H_2}$$

Therefore, there exists ψ such that

$$\rho(\delta+1) = \frac{\dot{n}_{EX} - \beta \delta}{\beta} = \dot{n}_{EX} - \dot{n}_{H_2} = 0$$

$$N^I = \frac{\partial \psi}{\partial t} = n^{\delta} (\dot{n}_{H_2} y - \dot{n}_{H_2})$$

$$\partial \psi = (\dot{n}_{H_2} y - \dot{n}_{H_2}) \int n^{\delta} dt$$

$$\psi = \frac{(\dot{n}_{H_2} y - \dot{n}_{H_2})}{\delta+1} [n^{\delta+1}]^{B-8} + h(y) = C$$

since $(\delta+1)\beta =$ n_{H_2}

$$\psi = (y-1)n^{\delta+1} + h(y) = C$$

Now taking $\frac{\partial \psi}{\partial y}$

$$\frac{\partial \psi}{\partial y} = n^{\delta+1} + h'(y)$$

and setting equal to $\frac{\partial \psi}{\partial y} = N^{\frac{\delta}{\delta+1}} n^{\delta+1}$

$$\therefore h'(y) = 0 \text{ and } h(y) = 0$$

Therefore, general sol'n :

$$n = \beta t + n^0$$

$$\psi = (y-1)n^{\delta+1} = C$$

and solving for C at initial conditions, $t=0$
 $y=y^0$

$$C = (y^0-1)n^{0\delta+1}$$

Therefore,

$$(y-1)n^{\delta+1} - (y^0-1)n^{0\delta+1} = 0$$

and solving for y,

$$(y-1) = \frac{n^{0\delta+1}}{n^{\delta+1}} (y^0-1)$$

$$y = \frac{n^{0\delta+1}}{n^{\delta+1}} (y^0-1) + 1$$

Time Delay - Problem 2

Overall Balancein: $\dot{n}_{H_2}$

out: 0

Accum: $\frac{dn}{dt} = \dot{n}_{H_2}$

$$n - n_0 = \dot{n}_{H_2} t$$

$$\therefore n = \dot{n}_{H_2} t + n_0$$

H₂ Balancein: $\dot{n}_{H_2}$

out: 0

Accum: $\frac{d(ny)}{dt}$

$$n \frac{dy}{dt} + y \frac{dn}{dt} = \dot{n}_{H_2}$$

$$n \frac{dy}{dt} + \dot{n}_{H_2} y - \dot{n}_{H_2} = 0$$

checking "exactness":

$$\frac{\partial M}{\partial y} = \dot{n}_{H_2} \quad \frac{\partial N}{\partial t} = \dot{n}_{H_2} \quad \text{exact}$$

Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = \dot{n}_{H_2} y - \dot{n}_{H_2}$$

$$\therefore \psi = \dot{n}_{H_2}(y-1)t + h(y) = c \quad \leftarrow \text{General Sol'n}$$

and

$$\frac{\partial \psi}{\partial y} = \dot{n}_{H_2} t + h'(y)$$

Setting equal to $\frac{\partial \psi}{\partial y} = \dot{n}_{H_2} t + n_0$

$$\therefore h'(y) = n_0 \quad \text{and} \quad h(y) = n_0 y$$

Substituting into General Sol'n:

$$\therefore \dot{n}_{H_2}(y-1)t + n_0 y = c$$

and solving for c , @ initial conditions $t=0$
 $y=y_0$

$$c = n_0 y_0$$

and substituting into General Sol'n:

$$\dot{n}_{H_2}(y-1)t + n_0 y = n_0 y_0$$

Now solving for y :

$$\dot{n}_{H_2} t y - \dot{n}_{H_2} t + n_0 y = n_0 y_0$$

$$y(\dot{n}_{H_2} t + n_0) = \dot{n}_{H_2} t + n_0 y_0$$

$$\therefore y = \frac{(\dot{n}_{H_2} t + n_0 y_0)}{(\dot{n}_{H_2} t + n_0)} \quad \text{B-11}$$

Pressure / Time Relationship:

$$n = \dot{n}_{H_2} t + n_0 = \frac{PV}{RT} \quad n_0 = \frac{P^0 V}{RT}$$

$$\begin{aligned} \therefore P &= \frac{RT}{V} (\dot{n}_{H_2} t + n_0) \\ &= \frac{RT}{V} (\dot{n}_{H_2} t + \frac{P^0 V}{RT}) \end{aligned}$$

$$\therefore P = \frac{RT}{V} \dot{n}_{H_2} t + P^0 \quad \dot{n}_{H_2} t = n - n_0$$

y in terms of P:

$$y = \frac{(\dot{n}_{H_2} t + n_0 y_0)}{(\dot{n}_{H_2} t + n_0)} = \frac{(n - n_0 + n_0 y_0)}{n}$$

$$y = 1 - \frac{n_0}{n} + \frac{n_0}{n} y_0$$

$$y = 1 + \frac{n_0}{n} (y_0 - 1)$$

$$y = 1 + \frac{P^0}{P} (y_0 - 1)$$

Appendix C

Problem 3 - Helium Purge

 $\dot{n}_i$ = interim gmol/min

 n_1 = total gmol in tank 1

 n_2 = total gmol in tank 2

 y_1 = helium fraction in tank 1

 y_2 = helium fraction in tank 2

assume T & P in both tanks = m

Overall Balance

Tank 1

 in: $\dot{n}_{He}$

 out: $\dot{n}_i$

Accum: 0 (steady state)

$$\therefore \dot{n}_{He} = \dot{n}_i$$

$$\therefore \dot{n}_i = \dot{n}_{He} = \dot{n}_{ex}$$

Tank 2

 in: $\dot{n}_i$

 out: $\dot{n}_{ex}$

Accum: 0 (steady state)

$$\dot{n}_i = \dot{n}_{ex}$$

Helium Balance (assuming remaining gas is air)

Tank 1

 in: $\dot{n}_{He}$

 out: $\dot{n}_i y_1$

 Accum: $\frac{d(n_1 y_1)}{dt}$

$$\therefore \frac{d(n_1 y_1)}{dt} = \dot{n}_{He} - \dot{n}_i y_1$$

$$n_1 \frac{dy_1}{dt} + y_1 \frac{dn_1}{dt} \stackrel{0}{=} \dot{n}_{He} - \dot{n}_i y_1$$

$$n_1 = \dot{n}_{He} C-2$$

Tank 2

 in: $\dot{n}_i y_1$

 out: $\dot{n}_{ex} y_2$

 Accum: $\frac{d(n_2 y_2)}{dt}$

$$\frac{d(n_2 y_2)}{dt} = \dot{n}_i y_1 - \dot{n}_{ex} y_2$$

Solving around Tank 1:

$$n_1 \frac{dy_1}{dt} = \dot{n}_{He} - \dot{n}_1 y_1$$

$$\dot{n}_1 = \frac{PV_1}{RT}$$

$$n_1 \frac{dy_1}{dt} + \dot{n}_{He} y_1 - \dot{n}_{He} = \dot{n}_{He} (y_1 - 1)$$

Solving for Integration Factor, μ

$$\frac{d\mu}{dt} = \frac{\dot{n}_{He}}{n_1} \mu$$

$$\ln \mu = \frac{\dot{n}_{He}}{n_1} t$$

$$\mu = e^{\dot{n}_{He} t / n_1}$$

Multiplying all terms by μ ,

$$n_1 e^{\dot{n}_{He} t / n_1} \frac{dy_1}{dt} + e^{\dot{n}_{He} t / n_1} (\dot{n}_{He} y_1 - \dot{n}_{He}) = 0$$

Therefore, there exists, ψ such that:

$$\frac{\partial \psi}{\partial t} = e^{\dot{n}_{He} t / n_1} (\dot{n}_{He} y_1 - \dot{n}_{He}) = \dot{n}_{He} e^{\dot{n}_{He} t / n_1} (y_1 - 1)$$

$$\psi = \frac{\dot{n}_{He} (y_1 - 1)}{\dot{n}_{He}} n_1 e^{\dot{n}_{He} t / n_1} + h(y_1)$$

$$\text{and } \frac{\partial \psi}{\partial y_1} = n_1 e^{\dot{n}_{He} t / n_1} + h'(y_1)$$

$$\text{and setting equal to } \frac{\partial \psi}{\partial y_1} = n_1 e^{\dot{n}_{He} t / n_1}$$

$$\therefore h'(y_1) = 0 \text{ and } h(y_1) = 0$$

and substituting into general sol'n:

$$(y_1 - 1) n_1 e^{\dot{n}_{He} t / n_1} = C$$

Solving for C , at initial conditions, $t=0$, $y_1 = y_1^0$

$$C = (y_1^0 - 1)n_1$$

Therefore,

$$(y_1 - 1) e^{n_1 t / n_1} = (y_1^0 - 1) e^{n_1 t / n_1}$$

and solving for y_1 :

$$y_1 = (y_1^0 - 1) e^{-n_1 t / n_1} + 1 \quad \text{let } \delta(t) = \frac{n_1 t}{n_1}$$

$$\therefore y_1 = (y_1^0 - 1) e^{-\delta(t)} + 1$$

Tank 2 Helium Balance

$$\frac{d(n_2 y_2)}{dt} = \underset{\substack{\uparrow \\ n_{ex}}}{n_1} y_1 - n_{ex} y_2 = n_{ex} (y_1 - y_2)$$

$$n_2 \frac{dy_2}{dt} + y_2 \frac{dn_2}{dt} \overset{ss}{=} n_{ex} (y_1 - y_2)$$

$$n_2 \frac{dy_2}{dt} - n_{ex} (y_1 - y_2) = 0$$

substituting exact solution for y_1 , $y_1 = (y_1^0 - 1) e^{-\delta(t)} + 1$

$$\therefore n_2 \frac{dy_2}{dt} - n_{ex} (1 + (y_1^0 - 1) e^{-\delta(t)}) + n_{ex} y_2 = 0$$

$$\frac{n_2}{n_{ex}} \frac{dy_2}{dt} - (1 + (y_1^0 - 1) e^{-\delta(t)}) + y_2 = 0$$

check for "exactness",

$$\frac{\partial M}{\partial y_2} = 1$$

$$\frac{\partial N}{\partial t} = 0$$

No + exact

therefore,

$$\frac{d\mu}{dt} = \left[\frac{\dot{n}_{ex}}{n_2} \right] \mu$$

$$\frac{d\mu}{\mu} = \frac{\dot{n}_{ex}}{n_2} dt$$

$$\mu = e^{\frac{\dot{n}_{ex}}{n_2} t}$$

$$\text{let } \phi(t) = \frac{\dot{n}_{ex} t}{n_2}$$

Multiplying all terms by μ ,

$$e^{\phi(t)} \frac{n_2}{\dot{n}_{ex}} \frac{dy_2}{dt} - e^{\phi(t)} [1 + (y_1 - 1)e^{-\phi(t)}] + e^{\phi(t)} y_2 = 0$$

checking "exactness",

$$\frac{\partial M}{\partial y_2} = e^{\phi(t)}$$

$$\frac{\partial N}{\partial t} = \frac{n_2 + \dot{n}_{ex}}{\dot{n}_{ex} n_2} e^{\phi(t)} -$$

exact

Go to page 5

note: $\dot{n}_i = \dot{n}_{ex} = \dot{n}_{in}$ (steady state)

$$P = 14.7 \text{ psia}$$

$$T = 10^\circ\text{C} \quad \leftarrow \text{PWC (Receiving Tanks) temperature}$$

$$V_1 = 160 \text{ gal (empty)}$$

$$V_2 \approx 190 \text{ gal (empty) with minimum 50 gal water for pumping mco}$$

$$\therefore \text{take } V_1 = 160 \text{ gal} \approx 20 \text{ ft}^3$$

$$V_2 = 190 - 50 = 140 \text{ gal} \approx 19 \text{ ft}^3$$

Therefore, there exists ϕ such that:

$$\phi = \frac{n_2 t}{n_1}$$

$$\delta = \frac{n_2 t}{n_1}$$

$$\frac{\partial \psi}{\partial t} = e^{\phi} y_2 - e^{\phi} (1 + (y_1^0 - 1)e^{\phi - \delta})$$

$$= e^{\phi} y_2 - e^{\phi} - (y_1^0 - 1)e^{\phi - \delta}$$

$$\frac{\partial \psi}{\partial t} = e^{\phi} (y_2 - 1) + (1 - y_1^0) e^{\phi - \delta}$$

$$\psi = \frac{n_2 (y_2 - 1)}{n_2} e^{\phi} + \frac{n_1 n_2 (1 - y_1^0)}{n_2 (n_1 - n_2)} e^{\phi - \delta} + h(y_2) = C$$

$$\frac{\partial \psi}{\partial y_2} = \frac{n_2}{n_2} e^{\phi} + h'(y_2) = C$$

Setting equal to $\frac{\partial \psi}{\partial y_2} = \frac{n_2}{n_2} e^{\phi} \therefore h'(y_2) = 0, h(y_2) = 0$

and solving for C , @ initial condition too
 $y_2 = y_2^0$

$$C = \frac{n_2 (y_2^0 - 1)}{n_2} + \frac{n_1 n_2 (1 - y_1^0)}{n_2 (n_1 - n_2)}$$

$$\frac{n_2}{n_2} \left[(y_2 - 1) e^{\phi} + \frac{n_1 (1 - y_1^0)}{(n_1 - n_2)} e^{\phi - \delta} \right] = \frac{n_2}{n_2} \left[(y_2^0 - 1) + \frac{n_1 (1 - y_1^0)}{(n_1 - n_2)} \right]$$

Solving for y_2

$$(y_2 - 1) = \left[(y_2^0 - 1) + \beta \right] e^{-\phi} - \frac{\beta e^{\phi - \delta}}{e^{\phi}}$$

$$y_2 = \left[(y_2^0 - 1) + \beta \right] e^{-\phi} - \beta e^{-\delta} + 1$$

Appendix D

Prob 4

1/2

$$n_2 = \frac{PV_2}{RT}$$

 $V_2 = \text{void vol Tank 2}$

- assume counter current (cc) equimolar flow

Air Balance

- assume no air escapes cc (conservative)

in: $\dot{n}_{air}$

out: 0

Accum: $\frac{d(n_2 y_2)}{dt}$ cc equimolar

$$n_2 \frac{dy_2}{dt} + y_2 \frac{dn_2}{dt} = \dot{n}_{air}$$

(Treybzt 1963)

$$\dot{n}_{air} = \frac{D_{air/m_2} A P}{RT_2} (y_2^0 - y_2)$$

$A \equiv$ CS. area of pipe leading into Tank 2

$y_2^0 = 1$ (air ingress fraction)

$$\frac{dy_2}{dt} = \frac{\dot{n}_{air}}{n_2} = \frac{D_{air/m_2} A P (y_2^0 - y_2) RT}{RT_2 PV_2}$$

$z \equiv$ pipe length of air ingress

$$= \frac{D_{air/m_2} A (y_2^0 - y_2)}{z V_2}$$

$$\text{let } \alpha = \frac{D_{air/m_2} A}{z V_2}$$

$$\frac{dy_2}{dt} = \alpha (y_2^0 - y_2)$$

$$\frac{dy_2}{(y_2^0 - y_2)} = \alpha dt$$

$$\text{let } u = (y_2^0 - y_2)$$

$$\frac{du}{dy_2} = -1 \quad \text{or } du = -dy_2$$

$$\therefore -\frac{du}{u} = \alpha dt$$

$$\ln u = -\alpha t + C$$

$$\ln(1 - y_2) = -\alpha t + C$$

Solving for C , @ initial conditions,

$$t=0$$

$$y_2^0 = 0$$

← pseudo steady state

$$\ln(1 - y_2^0) = C$$

$$\therefore C = 0$$

$$\therefore \ln(1 - y_2) = -\alpha t$$

and

$$(1 - y_2) = e^{-\alpha t}$$

$$\therefore y_2 = 1 - e^{-\alpha t}$$

and $\therefore$ the O_2 fraction, 21% air:

$$y_{O_2} = 0.21 y_2$$

Diffusion Coeff - Perry 6th Ed

$$D_{AB} = \frac{10^{-3} T^{1.75} [(M_A + M_B) / M_A M_B]^{1/2}}{P [(\Sigma V)_A^{1/3} + (\Sigma V)_B^{1/3}]^2}$$

pg 3-285

$$T \equiv K$$

$$P \equiv \text{atm}$$

$$D_{AB} \equiv \text{cm}^2/\text{sec}$$

$$M_A \text{ ; } M_B \equiv \text{MW of A, B, resp.}$$

$$(\Sigma V)_A \text{ and } (\Sigma V)_B \equiv \text{Table 3-342, pg 3-285}$$

$$\text{let } A = \text{air}$$

$$B = \text{helium}$$

$$\therefore M_{\text{air}} = 29 \text{ lbm/lbmol}$$

$$M_{\text{He}} = 4 \text{ lbm/lbmol}$$

$$T = 21^\circ\text{C} \text{ or } 294 \text{ K}$$

$$P = 1 \text{ atm}$$

$$(\Sigma V)_{\text{air}} = 20.1$$

$$(\Sigma V)_{\text{He}} = 2.88$$

$$\therefore D_{\text{air/He}} = \frac{10^{-3} (294)^{1.75} [(29+4)/29(4)]^{1/2}}{(1) [(20.1)^{1/3} + (2.88)^{1/3}]^2} = \frac{11.134}{17.154} = 0.649 \frac{\text{cm}^2}{\text{sec}}$$

Appendix E

Problem 5

12

Rate of heat loss from water = Rate of heat transfer thru tank steel = Rate of heat loss from outside tank

$$h_1 A (T - T_w) = \frac{kA}{l} (T_w - T_s) = h_2 A (T_s - T_{\infty})$$

T = bulk water temperature
in tank

T_w = inside tank wall temperature

h_1 = heat transfer coeff (water film)

A = area of water/inside tank interface
also, area of air/outside tank interface

assume $A_i = A_o = A$

k = thermal conductivity for steel (tank)

l = tank thickness

T_s = outside tank surface temperature

T_{∞} = temperature of ambient air outside tank

h_2 = heat transfer coeff at tank surface
convection

or $h_{2c} = h_2$

Rearranging 1st two terms, and solving for T_w :

$$h_1 A (T - T_w) = \frac{kA}{l} (T_w - T_s)$$

$$h_1 T - h_1 T_w = \frac{k}{l} T_w - \frac{k}{l} T_s$$

$$h_1 T + \frac{k}{l} T_s = \frac{k}{l} T_w + h_1 T_w = T_w \left(\frac{k}{l} + h_1 \right)$$

$$T_w = \frac{\left(h_1 T + \frac{k}{l} T_s \right)}{\left(\frac{k}{l} + h_1 \right)}$$

Substituting into last 2 terms and solving for T_s

$$\frac{kA}{l} (T_w - T_s) = h_2 A (T_s - T_{air})$$

$$T_w = \frac{h_2 l}{k} (T_s - T_{air}) + T_s$$

$$\text{set } T_w = T_w$$

$$\frac{(h_1 T + \frac{k}{l} T_s)}{(\frac{k}{l} + h_1)} = \frac{h_2 l}{k} (T_s - T_{air}) + T_s$$

$$h_1 T + \frac{k}{l} T_s = (\frac{k}{l} + h_1) \frac{h_2 l}{k} (T_s - T_{air}) + T_s (\frac{k}{l} + h_1)$$

$$\begin{aligned} \frac{k}{l} T_s - T_s (\frac{k}{l} + h_1) &= (h_2 + h_1 h_2 \frac{l}{k}) (T_s - T_{air}) - h_1 T \\ -T_s h_1 &= h_2 T_s + h_1 h_2 \frac{l}{k} T_s - T_{air} h_2 - h_1 h_2 \frac{l}{k} T_{air} - h_1 T \\ T_s h_1 + h_2 T_s + h_1 h_2 \frac{l}{k} T_s &= -T_{air} h_2 + h_1 h_2 \frac{l}{k} T_{air} + h_1 T \end{aligned}$$

$$T_s (h_1 + h_2 + h_1 h_2 \frac{l}{k}) = T_{air} (h_2 + h_1 h_2 \frac{l}{k}) + T h_1$$

$$T_s = \frac{[T_{air} (h_2 + h_1 h_2 \frac{l}{k}) + T h_1]}{(h_1 + h_2 + h_1 h_2 \frac{l}{k})}$$

$$T_s = \frac{T_{air} (h_2 + h_1 h_2 \frac{l}{k})}{(h_1 + h_2 + h_1 h_2 \frac{l}{k})} + T \frac{h_1}{(h_1 + h_2 + h_1 h_2 \frac{l}{k})}$$

$$T_s = a + bT \quad \begin{matrix} a = \\ E-3 \end{matrix} \frac{T_{air} (h_2 + h_1 h_2 \frac{l}{k})}{(h_1 + h_2 + h_1 h_2 \frac{l}{k})} \quad b = \frac{h_1}{(h_1 + h_2 + h_1 h_2 \frac{l}{k})}$$

Thermal Equilibrium of the Water (System)

3

Input Rate

Output Rate: $h_2 A (T_s - T_{2in})$ Accum: $m C_p \frac{dT}{dt}$

Accum = in - out

 $m_{\text{water}} (V_{\text{water}})_{\text{in tank}}$

- assume constant density

$$m C_p \frac{dT}{dt} = -h_2 A (T_s - T_{2in})$$

$$\text{where } T_s = a + bT$$

$$\frac{dT}{dt} = \frac{-h_2 A}{m C_p} (a + bT - T_{2in})$$

$$\text{Let } \beta = \frac{h_2 A}{m C_p} \quad (\equiv \text{hr}^{-1})$$

note: don't confuse
ht β with mass transfer

$$\frac{dT}{dt} = -\beta a - \beta b T + \beta T_{2in}$$

$$\frac{dT}{dt} = -\beta b T - \beta a + \beta T_{2in}$$

$$+ \underbrace{(\beta T_{2in} - \beta a)}_c \quad c = \beta (T_{2in} - a)$$

$$\text{let } c = \beta (T_{2in} - a) \\ = \frac{F}{\text{hr}}$$

$$\frac{dT}{dt} + \beta b T - c = 0$$

Need Integrating Factor, μ

$$\frac{\partial \mu}{\partial T} = \beta b$$

$$\frac{d\mu}{dt} = +\beta b \mu$$

$$\frac{d\mu}{\mu} = +\beta b dt$$

$$\ln \mu = +\beta b t$$

$$\mu = e^{+\beta b t}$$

Multiplying all terms by μ , or $e^{+\beta b t}$

$$e^{+\beta b t} \frac{dT}{dt} + e^{+\beta b t} \beta b T - c e^{+\beta b t} = 0$$

Therefore, there exists ψ such that,

$$\frac{\partial \psi}{\partial t} = +\beta \delta T e^{+\beta \delta t} - C e^{+\beta \delta t}$$

$$\psi = T e^{+\beta \delta t} - \frac{C}{\beta \delta} e^{+\beta \delta t} + h(T) = C_1 \quad \text{general sol'n}$$

$$\frac{\partial \psi}{\partial T} = e^{+\beta \delta t} + h'(T)$$

$$\text{Setting equal to } \frac{\partial \psi}{\partial T} = e^{+\beta \delta t} \quad \therefore \begin{aligned} h'(T) &= 0 \\ h(T) &= 0 \end{aligned}$$

into general sol'n:

$$\therefore T e^{+\beta \delta t} - \frac{C}{\beta \delta} e^{+\beta \delta t} = C_1$$

Solving for C_1 , @ initial conditions

$$t=0$$

$$T = T_0 (= 50^\circ \text{C})$$

$$\therefore C_1 = T_0 - \frac{C}{\beta \delta}$$

and substituting into general solution,

$$T e^{+\beta \delta t} - \frac{C}{\beta \delta} e^{+\beta \delta t} = T_0 - \frac{C}{\beta \delta}$$

and solving for T :

$$T e^{+\beta \delta t} = T_0 - \frac{C}{\beta \delta} + \frac{C}{\beta \delta} e^{+\beta \delta t}$$

$$T = T_0 e^{-\beta \delta t} - \frac{C}{\beta \delta} e^{-\beta \delta t} + \frac{C}{\beta \delta} = e^{-\beta \delta t} \left(T_0 - \frac{C}{\beta \delta} \right) + \frac{C}{\beta \delta}$$

↑ remember

$T_{\text{air}} = T_{\text{water in tank}}$

Overall Balance Around PWC Tanks (Mass)

Tank 1

in: $\dot{n}_i$

out: 0

Accum: $\frac{dn_1}{dt}$

$$\frac{dn_1}{dt} = \dot{n}_i - 0$$

$$\therefore \frac{dn_1}{dt} = \dot{n}_i$$

Tank 2

in: $\dot{n}_{2in}$

out: $\dot{n}_i$

Accum: $\frac{dn_2}{dt}$

$$\frac{dn_2}{dt} = \dot{n}_{2in} - \dot{n}_i$$

Assuming each tank loses heat equally, $T_1 = T_2$, since assuming same volume of water in each tank at same initial temperature. Both tanks same geometry regarding containing water.

$$\therefore \frac{P}{RT} = \frac{n_1}{V_1} = \frac{n_2}{V_2}$$

$$n_1 = \frac{V_1}{V_2} n_2 \quad k = \frac{V_1}{V_2}$$

$$n_1 = k n_2$$

$$\therefore \frac{dn_1}{dt} = k \frac{dn_2}{dt}$$

$$\frac{dn_2}{dt} = \dot{n}_{2in} - \frac{dn_1}{dt}$$

$$\text{and since } \frac{dn_1}{dt} = k \frac{dn_2}{dt}$$

$$\frac{dn_2}{dt} = \dot{n}_{2in} - k \frac{dn_2}{dt}$$

$$(1+k) \frac{dn_2}{dt} = \dot{n}_{2in}$$

$$dn_2 = \frac{\dot{n}_{2in}}{(1+k)} dt$$

$$\text{let } \beta = \frac{\dot{n}_{2in}}{(1+k)}$$

$$n_2 = \beta t + n_2^0$$

and since $n_1 = k n_2$ $n_2 = \frac{1}{k} n_1$ $n_2^0 = \frac{1}{k} n_1^0$

$$\frac{1}{k} n_1 = \frac{\dot{n}_{21} t}{(1+k)} + \frac{1}{k} n_1^0$$

or

$$n_1 = \frac{k \dot{n}_{21} t}{(1+k)} + n_1^0$$

let $\alpha = \frac{k \dot{n}_{21}}{(1+k)} = k\beta$

$$\therefore n_1 = \alpha t + n_1^0 \quad n_2 = \beta t + n_2^0$$

$$\beta = \frac{\dot{n}_{21}}{(1+k)}$$

$$\therefore \frac{dn_1}{dt} = \alpha$$

$$\frac{dn_2}{dt} = \beta$$

$$\dot{n}_1 = \frac{dn_1}{dt} = \alpha$$

Air Balance Around PWC Tanks

Tank 2

in: $\dot{n}_{21}$

out: $\dot{n}_2 y_2$

Accum: $\frac{d(n_2 y_2)}{dt}$

$$n_2 \frac{dy_2}{dt} + y_2 \frac{dn_2}{dt} = \dot{n}_{21} - \dot{n}_2 y_2$$

$$n_2 \frac{dy_2}{dt} + y_2 \beta = \dot{n}_{21} - \alpha y_2$$

$$n_2 \frac{dy_2}{dt} + y_2 (\beta + \alpha) - \dot{n}_{21} = 0$$

$$\beta + \alpha = \beta + k\beta = \beta(1+k)$$

$$n_2 \frac{dy_2}{dt} + \beta(1+k) y_2 - \dot{n}_{21} = 0$$

checking "exactness"

$$\frac{\partial M}{\partial y_2} = \beta(1+k)$$

$$\frac{\partial N}{\partial t} = \beta$$

E-7

not exact

Therefore, need Integration Factor μ

$$\frac{d\mu}{dt} = \frac{(\beta + \beta k - \beta)}{n_2} \mu = \frac{\beta k}{n_2} \mu$$

$$\frac{d\mu}{\mu} = \frac{\beta k dt}{n_2}$$

$$n_2 = \beta t + n_2^0$$

$$\ln \mu = - \frac{\beta k}{\beta} \ln n_2$$

$$\mu = n_2^k$$

$\therefore$ Multiply all terms by μ

$$n_2^{1+k} \frac{dy_2}{dt} + n_2^k y_2 \beta (1+k) - n_2^k i_{2in} = 0$$

checking "exactness"

$$\frac{\partial M^+}{\partial y_2} = \beta (1+k) n_2^k -$$

$$\frac{\partial N^+}{\partial y_2} = (1+k) n_2^k \beta - \text{exact}$$

Therefore, there exists ψ such that,

$$\frac{\partial \psi}{\partial t} = n_2^k y_2 \beta (1+k) - n_2^k i_{2in} = n_2^k [y_2 \beta (1+k) - i_{2in}]$$

$$\psi = \frac{(y_2 \beta (1+k) - i_{2in}) n_2^{1+k}}{(1+k) \beta} + h(y_2) = C$$

or

$$\psi = \left(y_2 - \frac{i_{2in}}{\beta (1+k)} \right) n_2^{1+k} + h(y_2) = C$$

$$\frac{\partial \psi}{\partial y_2} = n_2^{1+k} + h'(y_2)$$

$$\text{Setting equal to } \frac{\partial \psi}{\partial y_2} = n_2^{1+k}$$

$$\therefore h'(y_2) = 0 \text{ and } h(y) = 0$$

Substituting into general solution:

$$\left(y_2 - \frac{n_{21r}}{\beta(1+k)}\right) n_2^{1+k} = C$$

and solving for C, @ initial conditions, $t=0$
 $y_2 = y_2^0$

$$C = \left(y_2^0 - \frac{n_{21r}}{\beta(1+k)}\right) n_2^0^{1+k}$$

Therefore, solution is:

$$\left(y_2 - \frac{n_{21r}}{\beta(1+k)}\right) n_2^{1+k} = \left(y_2^0 - \frac{n_{21r}}{\beta(1+k)}\right) n_2^0^{1+k}$$

and solving for y_2 :

$$y_2 - \frac{n_{21r}}{\beta(1+k)} = \left(\frac{n_2^0}{n_2}\right)^{1+k} \left(y_2^0 - \frac{n_{21r}}{\beta(1+k)}\right)$$

$$y_2 = \left(\frac{n_2^0}{n_2}\right)^{1+k} \left(y_2^0 - \frac{n_{21r}}{\beta(1+k)}\right) + \frac{n_{21r}}{\beta(1+k)}$$

where: $n_2^0 = \frac{PV_2}{RT^0}$ and $n_2 = \frac{PV_2}{RT}$

$$\frac{n_2^0}{n_2} = \frac{1/T^0}{1/T} = \frac{T}{T^0}$$

$$y_2 = \left(\frac{T}{T^0}\right)^{1+k} \left(y_2^0 - \frac{n_{21r}}{\beta(1+k)}\right) + \frac{n_{21r}}{\beta(1+k)} \quad \leftarrow \text{since } \beta = \frac{n_{21r}}{(1+k)}$$

$$y_2 = \left(\frac{T}{T^0}\right)^{1+k} (y_2^0 - 1) + 1 \quad \leftarrow \text{Solution to } y_2$$

Air Balance Around Tank 1in: $n_1 y_2$ $n_1 = L$

$$\alpha = \frac{k n_{20}}{(k+1)} = k\beta$$

out: 0

Accum: $\frac{d(n_1 y_1)}{dt}$

$$\frac{dn_1}{dt} = L$$

$$n_1 = Lt + n_1^0$$

$$\frac{d(n_1 y_1)}{dt} = n_1 y_2$$

$$n_1 \frac{dy_1}{dt} + y_1 \frac{dn_1}{dt} = L y_2$$

$$n_1 \frac{dy_1}{dt} + L y_1 = L y_2$$

$$n_1 \frac{dy_1}{dt} + L y_1 - L y_2 = 0$$

$$y_2 = \left(\frac{n_{20}}{n_2} \right)^{k+1} (y_2^0 - 1) + 1$$

$$n_1 \frac{dy_1}{dt} + L y_1 - L \left[\left(\frac{n_{20}}{n_2} \right)^{k+1} (y_2^0 - 1) + 1 \right] = 0$$

checking "exactness"

$$\frac{\partial M}{\partial y_1} = L$$

$$\frac{\partial N}{\partial t} = L$$

✓ exact

∴ Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = L y_1 - L \left[\left(\frac{n_{20}}{n_2} \right)^{k+1} (y_2^0 - 1) + 1 \right]$$

$$\frac{\partial \psi}{\partial t} = L y_1 - L \left(\frac{n_{20}}{n_2} \right)^{k+1} (y_2^0 - 1) - L$$

$$\psi = \alpha(y_1 - 1)t - \alpha(y_2^0 - 1)n_2^0 \int n_2^{-(k+1)} dt$$

$$n_2 = \beta t + n_2^0$$

$$\int (a + bt)^n dt = \frac{(a + bt)^{n+1}}{(n+1)b}$$

$$\text{let } n = -(k+1)$$

$$n+1 = -k-1+1 = -k$$

$$a = n_2^0$$

$$b = \beta$$

$$= \frac{n_2^{-k}}{-k\beta} = \frac{n_2^{-k}}{-\alpha}$$

general solution

$$\psi = \alpha(y_1 - 1)t - \alpha(y_2^0 - 1)n_2^0 \left(\frac{n_2^{-k}}{-k} \right) + h(y_1) = C$$

$$\psi = \alpha(y_1 - 1)t + (y_2^0 - 1) \frac{n_2^{k+1}}{n_2^k} + h(y_1) = C$$

and

$$\frac{\partial \psi}{\partial y_1} = \alpha t + h'(y_1) \quad \text{Setting equal to } \frac{\partial \psi}{\partial y_1} = \alpha t + n_1^0$$

$$\therefore h'(y_1) = n_1^0 \quad \text{and} \quad h(y_1) = n_1^0 y_1$$

Substituting into general solution,

$$\alpha(y_1 - 1)t + (y_2^0 - 1) \frac{n_2^{k+1}}{n_2^k} + n_1^0 y_1 = C$$

and solving for C, at initial conditions, $t=0$
 $y_1 = y_1^0$

$$C = (y_2^0 - 1)n_2^0 + n_1^0 y_1^0$$

$\therefore$ solution is:

$$\alpha(y_1 - 1)t + (y_2^0 - 1) \frac{n_2^{k+1}}{n_2^k} + n_1^0 y_1 = (y_2^0 - 1)n_2^0 + n_1^0 y_1^0$$

and solving for y_1 :

$$y_1(\underbrace{\Delta t + n_1^0}_{n_1}) - \Delta t = (y_2^0 - 1)n_2^0 + n_1^0 y_1^0 - (y_2^0 - 1) \frac{n_2^0}{n_2^k} \Delta t$$

$$y_1 n_1 = (y_2^0 - 1)n_2^0 + n_1^0 y_1^0 - (y_2^0 - 1) \frac{n_2^0}{n_2^k} \Delta t + \Delta t$$

$$y_1 n_1 = (y_2^0 - 1)n_2^0 \left(1 - \frac{n_2^0}{n_2^k}\right) + n_1^0 y_1^0 + \Delta t$$

$$y_1 = (y_2^0 - 1) \left(1 - \left(\frac{n_2^0}{n_2}\right)^k\right) \frac{n_2^0}{n_1} + \frac{n_1^0}{n_1} y_1^0 + \frac{\Delta t}{n_1}$$

$$\left(\frac{n_2^0}{n_2}\right)^k = \left(\frac{T}{T^0}\right)^k \quad \frac{n_1^0}{n_1} = \frac{T}{T^0}$$

$$n_2 = k n_1$$

$$\frac{n_2^0}{n_1} = \frac{k^{1/2} / RT^0}{k^{1/2} / RT} = \frac{1/T^0}{k/T} = \frac{T}{kT^0}$$

$$\frac{n_1}{n_1} = \frac{\Delta t + n_1^0}{n_1} \quad \therefore \frac{\Delta t}{n_1} = 1 - \frac{n_1^0}{n_1} = 1 - \frac{T}{T^0}$$

$$y_1 = \left(\frac{T}{kT^0}\right) \left(1 - \left(\frac{T}{T^0}\right)^k\right) (y_2^0 - 1) + \frac{T}{T^0} y_1^0 + 1 - \frac{T}{T^0}$$

$$y_1 = \left(\frac{T}{kT^0}\right) \left(1 - \left(\frac{T}{T^0}\right)^k\right) (y_2^0 - 1) + \frac{T}{T^0} (y_1^0 - 1) + 1$$

For vertical cylinders: where $1 < Pr < 40$
in air

$$Pr = \frac{C_p \mu}{k}$$

$$Pr_{air @ 133^\circ C} = 0.69$$

$C_{p,air @ 212^\circ F}$: from McCabe/Smith pg 936
 (70°F) 4th Ed

$$@ 70^\circ F \quad C_{p,air} = 0.52 \frac{Btu}{lb_m \cdot ^\circ F}$$

$\mu_{air @ 70^\circ F}$:

$$@ 70^\circ F \quad \mu_{air} = 0.018 \text{ cP}$$

from McCabe/Smith pg 929
 4th Ed

$$1 \text{ cP} = 2.42 \frac{lb_m}{ft \cdot h} \quad (\text{see pg 41})$$

$$air \quad k @ 32^\circ F = 0.0140$$

$$air \quad k @ 212^\circ F = 0.0184$$

from McCabe/Smith pg 933
 4th Ed

So determining linearly,

$$T = 32 \quad k = 0.0140$$

$$T = 70 \quad k_{70} = ? = 0.0150$$

$$T = 212 \quad k = 0.0184$$

$$k_{air @ 70^\circ F} = 0.015 \frac{Btu}{ft \cdot h \cdot ^\circ F}$$

$$\frac{0.0184 - 0.0140}{212 - 32} = \frac{k - 0.0140}{70 - 32}$$

$$k = 0.0150$$

$$\therefore Pr = \frac{C_p \mu}{k} = \frac{(0.52)(0.018)(2.42)}{(0.015)} = \underline{\underline{1.51}}$$

checking,

$$\frac{\left(\frac{Btu}{lb_m \cdot ^\circ F} \right) \left(\frac{lb_m}{ft \cdot h} \right)}{\left(\frac{Btu}{ft \cdot h \cdot ^\circ F} \right)}$$

$$Gr = \frac{L^3 \rho^2 \beta g \Delta T}{\mu^2} \quad \text{-- see page 325 M'olz/Smith}$$

$$\beta = \frac{1}{T} = \frac{1}{(460 + 70) R} = \frac{1}{530 R} = 1.887 \times 10^{-3} R^{-1}$$

Tanks cylindrical with cone bottoms (assume all cylinders)

Tank 1: 160 gal total

inside dia (both)

Tank 2: 175 gal

outside: 23.5" + thickness(2)

say $\frac{1}{2}$ " thickness

$$V = Area \times Length$$

$$= \frac{\pi}{4} D^2 \times L$$

$$= \frac{\pi}{4} (dia + 2 \times thickness)^2 \times L$$

$$A_1 = A_2$$

$$A_1 = \frac{V_1}{L_1}$$

$$V = 3.274 \times L$$

$$\text{Tank 1: } L_1 = \frac{V_1}{3.274 \text{ ft}^2} = \frac{160 \text{ gal} \times \frac{1 \text{ ft}^3}{7.4805 \text{ gal}}}{3.274 \text{ ft}^2} = 6.5 \text{ ft}$$

$$\text{Tank 2: } L_2 = L_1 \left(\frac{V_2}{V_1} \right) = 6.5 \text{ ft} \left(\frac{175}{160} \right) = 7.1 \text{ ft}$$

Assume: $L = 5 \text{ ft}$ full of water -- both tanks

$$L^3 = 5^3 = \underline{125 \text{ ft}^3}$$

$$P_{air} = \frac{n}{V} = \frac{P}{RT} =$$

$$R = 0.04259 \frac{\text{psia} \cdot \text{ft}^3}{\text{lbmol} \cdot \text{R}}$$

$$P_{air} = \frac{14.696 \text{ psia}}{\left(\frac{10.71 \text{ psia} \cdot \text{ft}^3}{\text{lbmol} \cdot \text{R}} \right) (530 \text{ R})}$$

$$= 0.00259 \frac{\text{lbmol}}{\text{ft}^3}$$

$$R = \frac{10.71 \text{ psia} \cdot \text{ft}^3}{\text{lbmol} \cdot \text{R}}$$

$$\therefore C^2 = 6.7 \times 10^6 \frac{\text{lbmol}^2}{\text{ft}^6}$$

$$g = 32.2 \frac{\text{ft}}{\text{sec}^2} \times \left(\frac{3600 \text{ sec}}{1 \text{ hr}} \right)^2 = 417,312,000 = 4.17 \times 10^8 \frac{\text{ft}}{\text{hr}^2}$$

$$\Delta T = (50 - 21)^\circ \text{C} = 7(582 - 529)^\circ \text{R} = 52^\circ \text{R}$$

$\nwarrow 70^\circ \text{F}$ $\nwarrow$ need in $^\circ \text{R}$

$$M = 0.018 \text{ CR} \times 2.42 \frac{\text{lbm}}{\text{ft} \cdot \text{h}} \bigg/ \text{CP} = 0.0436 \frac{\text{lbm}}{\text{ft} \cdot \text{h}}$$

$$M^2 = 0.001897 \approx 0.0019 \frac{\text{lbm}^2}{\text{ft}^2 \cdot \text{h}^2}$$

$$G_r = \frac{(125 \text{ ft}^3) (6.7 \times 10^6 \frac{\text{lbmol}^2}{\text{ft}^6}) \left(1 \frac{52^\circ \text{R}}{530^\circ \text{R}} \right) (4.17 \times 10^8 \frac{\text{ft}}{\text{hr}^2})}{0.0019 \frac{\text{lbm}^2}{\text{ft}^2 \cdot \text{h}^2}}$$

$$= 1.8 \times 10^7 \frac{\text{lbmol}^2}{\text{lbm}^2} \times \left(\frac{29 \text{ lbm}}{\text{lbmol}} \right)^2$$

$$\therefore \underline{G_r = 1.5 \times 10^{10}}$$

Appendix F

Problem 6

PWC POST PURGE

° need total gas H_2 during drain cycle for initial H_2 concentration

$$\text{Total } H_2 \text{ during drain: } \eta_{H_2}^0 = \eta_{H_2} \times 45 \text{ minutes}$$

Nominal MCO bulk water drain: 150 gal

Flush water: 80 gal

Total vol: 230 gal to PWC Tanks

Assume each PWC tank receives 115 gal

$$\text{Therefore, Tank 1 void space} = 160 - 115 = 45 \text{ gal} \\ \therefore V_1 = 6 \text{ ft}^3 \quad \text{or } \underline{6 \text{ ft}^3}$$

$$\text{Tank 2 void space} = 175 - 115 = 60 \text{ gal} \\ V_2 = 8 \text{ ft}^3 \quad \text{or } \underline{8 \text{ ft}^3}$$

Assume initial H_2 from MCO gas is transferred equally to both PWC Tanks:

Therefore:

$$\text{High Nominal } H_2 \text{ rate: } 6.4 \times 10^{-4} \text{ g/sec} \\ \text{or}$$

$$0.0192 \frac{\text{gmol } H_2}{\text{min}} \times 45 \text{ min} = 0.864 \text{ gmol } H_2 \quad \text{or } 0.0192 \frac{\text{gmol}}{\text{min}}$$

Initial PWC Tank mass (gmol):

$$\eta_1^0 = \frac{PV_1}{RT}$$

$$\eta_2^0 = \frac{PV_2}{RT}$$

$$T = 50^\circ\text{C} = 323 \text{ K}$$

$$P = 14.7 \text{ psia}$$

$$R = 0.04259 \frac{\text{psia} \cdot \text{ft}^3}{\text{gmol} \cdot ^\circ\text{K}} \quad \text{F-2}$$

$$\therefore n_1^0 = \frac{(14.7 \text{ psia})(6 \text{ ft}^3)}{(0.04259 \frac{\text{psia} \cdot \text{ft}^3}{\text{gmol} \cdot \text{K}})(323 \text{ K})} = 6.41 \text{ gmol}$$

$$n_2^0 = \frac{1}{K} n_1^0 = \left(\frac{8.0}{6.0} \right) 6.41 \text{ gmol} \quad n^0 = K n_2^0 \quad K = \frac{V_1}{V_2}$$

$$n_2^0 = 8.55 \text{ gmol}$$

Since H_2 equally dispersed, $y_{\text{H}_2}^0 = y_1^0 = y_2^0$

$$y_{\text{H}_2}^0 = \frac{n_{\text{H}_2}^0}{n_T^0} = \frac{n_{\text{H}_2}^0}{n_1^0 + n_2^0 + n_{\text{H}_2}^0} = \frac{0.864 \text{ gmol H}_2}{(6.41 + 8.55) + 0.864 \text{ gmol total}}$$

$$y_{\text{H}_2}^0 = 0.06 \quad \frac{\text{gmol H}_2}{\text{gmol gas in PWC tank}}$$

initial He mol fraction: $y_1^0 = 1 - y_{\text{H}_2}^0 = y_2^0$
in each Tank

Bounding case:

$$\text{H}_2/\text{min} = 2.4 \times 10^{-3} \text{ g/sec}$$

$$\text{or} \\ 0.072 \text{ gmol/min}$$

$$0.072 \frac{\text{gmol}}{\text{min}} \text{ H}_2 \times 45 \text{ min} = 3.24 \text{ gmol H}_2$$

$$\therefore y_{\text{H}_2}^0 = \frac{n_{\text{H}_2}^0}{n_T^0} = \frac{3.24 \text{ gmol H}_2}{(6.41 + 8.55 + 3.24) \text{ gmol total}} = \frac{0.18 \text{ gmol H}_2}{\text{gmol total}}$$

Overall BalanceTank 1in: $\dot{n}_{he}$ out: $\dot{n}_i$ Accum: $\frac{d\dot{n}_1}{dt} = 0$ since $\dot{n}_{he} = \dot{n}_i$

Assume SS

Tank 2in: $\dot{n}_i$ out: $\dot{n}_{ex}$ Accum: $\frac{d\dot{n}_2}{dt} = 0$ since $\dot{n}_i = \dot{n}_{ex}$ Helium BalanceTank 1in: $\dot{n}_{he}$ out: $\dot{n}_i y_1$ Accum: $\frac{d(\dot{n}_1 y_1)}{dt}$

$$\dot{n}_1 \frac{dy_1}{dt} + y_1 \frac{d\dot{n}_1}{dt} = \dot{n}_{he} - \dot{n}_i y_1$$

$$\dot{n}_1 \frac{dy_1}{dt} = \dot{n}_{he} - \dot{n}_{he} y_1$$

$$\dot{n}_1 \frac{dy_1}{dt} + \dot{n}_{he} (y_1 - 1) = 0$$

Tank 2in: $\dot{n}_i y_1$ out: $\dot{n}_{ex} y_2$ Accum: $\frac{d(\dot{n}_2 y_2)}{dt}$

$$\dot{n}_2 \frac{dy_2}{dt} + y_2 \frac{d\dot{n}_2}{dt} = \dot{n}_i y_1 - \dot{n}_{ex} y_2$$

- need integration factor, $\mu = e^{\frac{\dot{n}_1 t}{n_1}} = e^{rt}$ let $r = \frac{\dot{n}_1}{n_1}$

Multiplying all terms by μ ,

$$n_1 e^{rt} \frac{dy_1}{dt} + \dot{n}_1 e^{rt} (y_1 - 1) = 0$$

checking "exactness" $\frac{\partial M}{\partial y_1} = \dot{n}_1 e^{rt} \quad \frac{\partial N}{\partial t} = \dot{n}_1 e^{rt}$

Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = \dot{n}_1 e^{rt} (y_1 - 1)$$

general sol'n $\psi = \frac{\dot{n}_1 (y_1 - 1)}{r} e^{rt} = \frac{\dot{n}_1 (y_1 - 1)}{\dot{n}_1} n_1 e^{rt} = n_1 (y_1 - 1) e^{rt} + h(y_1) = C$

and

$$\frac{\partial \psi}{\partial y_1} = n_1 e^{rt} + h'(y_1)$$

Setting equal to $\frac{\partial \psi}{\partial y_1} = n_1 e^{rt}$

$$\therefore h'(y_1) = 0 \text{ and } h(y_1) = 0$$

Substituting into general solution:

$$n_1 (y_1 - 1) e^{rt} = C$$

Solving for C , at initial conditions, $t=0$
 $y_1 = y_1^0$

$$C = n_1 (y_1^0 - 1)$$

$\therefore$

$$n_1 (y_1 - 1) e^{rt} = n_1 (y_1^0 - 1)$$

and solving for y_1 :

$$(y_1 - 1) = e^{-rt} (y_1^0 - 1)$$

$$y_1 = e^{-rt} (y_1^0 - 1) + 1$$

$$r = \frac{\dot{n}_1}{n_1}$$

Proble

if $V_1 \neq V_2$

HNF-4301, Rev. 2

Task 2

$$n_2 \frac{dy_2}{dt} = \dot{n}_{He} y_1 - \dot{n}_{He} y_2$$

$$f = \frac{\dot{n}_{He}}{n_1}$$

$$y_1 = e^{-\tau t} (y_1^0 - 1) + 1$$

$$n_2 \frac{dy_2}{dt} - \dot{n}_{He} [e^{-\tau t} (y_1^0 - 1) + 1] + \dot{n}_{He} y_2 = 0$$

$$\frac{n_2}{\dot{n}_{He}} \frac{dy_2}{dt} - e^{-\tau t} \underbrace{(y_1^0 - 1)}_a - 1 + y_2 = 0$$

$$\frac{n_2}{\dot{n}_{He}} \frac{dy_2}{dt} - a e^{-\tau t} + y_2 - 1 = 0$$

$$\frac{\partial M^\pi}{\partial y_2} = 1$$

$$\frac{\partial N^\pi}{\partial t} = 0$$

$$\frac{d\mu}{dt} = \frac{\dot{n}_{He}}{n_2} \mu$$

$$\text{let } \phi = \frac{\dot{n}_{He}}{n_2}$$

$$\ln \mu = \phi t$$

$$\mu = e^{\phi t}$$

$$\frac{e^{\phi t}}{\phi} \frac{dy_2}{dt} - a e^{(\phi - \tau)t} + (y_2 - 1) e^{\phi t} = 0$$

checking "envelopes"

$$\frac{\partial M^\pi}{\partial y_2} = e^{\phi t} - \frac{\partial N^\pi}{\partial t} = e^{\phi t} -$$

$$\frac{\partial \psi}{\partial t} = (y_2 - 1)e^{\phi t} - a e^{(\phi - \delta)t}$$

$$\psi = \frac{(y_2 - 1)}{\phi} e^{\phi t} - \frac{a}{(\phi - \delta)} e^{(\phi - \delta)t} + h(y_2) = C$$

$$\frac{\partial \psi}{\partial y_2} = \frac{e^{\phi t}}{\phi} + h'(y_2) [=] \frac{e^{\phi t}}{\phi}$$

$$\therefore h'(y_2) = 0 \text{ and } h(y_2) = 0$$

$$\frac{(y_2 - 1)}{\phi} e^{\phi t} - \frac{a}{(\phi - \delta)} e^{(\phi - \delta)t} = C$$

$$e^{t=0} \\ y_2 = y_2^0$$

$$a = (y_2^0 - 1)$$

$$\frac{(y_2^0 - 1)}{\phi} - \frac{a}{(\phi - \delta)} = C$$

$$\delta t \quad \phi t - \delta t \neq 0 \dots$$

$$\frac{(y_2 - 1)}{\phi} e^{\phi t} - \frac{\phi a}{(\phi - \delta)} e^{(\phi - \delta)t} = \frac{(y_2^0 - 1)}{\phi} - \frac{a \phi}{(\phi - \delta)}$$

$$y_2 = e^{-\phi t} (y_2^0 - 1) - \frac{a \phi}{(\phi - \delta)} e^{-\phi t} + \frac{a \phi}{(\phi - \delta)} e^{-\delta t} + 1$$

$$y_2 = (y_2^0 - 1)e^{-\phi t} + \frac{a \phi}{(\phi - \delta)} [e^{-\delta t} - e^{-\phi t}] + 1$$

$$y_2 = (y_2^0 - 1)e^{-\phi t} + \frac{(y_2^0 - 1)\phi}{(\phi - \delta)} [e^{-\delta t} - e^{-\phi t}] + 1$$

if $V_1 \neq V_2$

Prob 6

if $V_1 = V_2$

$$\therefore n = n_1 = n_2$$

$$\dot{n}_{He} = \dot{n}_{Ox}$$

$$n \frac{dy_2}{dt} = \dot{n}_{He} y_1 - \dot{n}_{He} y_2$$

$$y_1 = e^{-\delta t} (y_1^0 - 1) + 1$$

$$\delta = \frac{\dot{n}_{He}}{n_1} = \frac{\dot{n}_{He}}{n}$$

$$n \frac{dy_2}{dt} - \dot{n}_{He} [e^{-\delta t} (y_1^0 - 1) + 1] + \dot{n}_{He} y_2 = 0$$

$$\frac{1}{\dot{n}_{He}} \frac{dy_2}{dt} - e^{-\delta t} (y_1^0 - 1) - 1 + y_2 = 0$$

$$\text{let } a = (y_1^0 - 1)$$

$$\frac{1}{\delta} \frac{dy_2}{dt} - a e^{-\delta t} + (y_2 - 1) = 0$$

$$\frac{\partial M}{\partial y_2} = 1$$

$$\frac{\partial N}{\partial t} = 0$$

$$\frac{dM}{dt} = \delta M$$

$$\text{or } \ln M = \delta t$$

$$M = e^{\delta t}$$

$$\frac{e^{\delta t}}{\delta} \frac{dy_2}{dt} - a + e^{\delta t} (y_2 - 1) = 0$$

checking exactness!

$$\frac{\partial M^0}{\partial y_2} = e^{\delta t} - \frac{\partial N^0}{\partial t} = e^{\delta t} -$$

$$\frac{\partial \psi}{\partial t} = e^{\delta t} (y_2 - 1) - a$$

$$\psi = \frac{(y_2 - 1)}{\delta} e^{\delta t} - a t + h(y_2) = c$$

$$\frac{\partial \psi}{\partial y_2} = \frac{e}{\delta} + h'(y_2) = \frac{e}{\delta}$$

$$h'(y_2) = 0 \text{ and } h(y_2) = 0$$

$$\frac{(y_2 - 1)}{\delta} e^{\delta t} - at = c$$

$$t=0 \\ y_2 = y_2^0$$

$$\frac{(y_2^0 - 1)}{\delta} = c$$

$$\therefore \frac{(y_2 - 1)}{\delta} e^{\delta t} - at = \frac{(y_2^0 - 1)}{\delta}$$

$$(y_2 - 1) e^{\delta t} - \delta at = (y_2^0 - 1)$$

$$(y_2 - 1) = e^{-\delta t} (y_2^0 - 1) + \delta at e^{-\delta t}$$

$$y_2 = e^{-\delta t} (y_2^0 - 1) + \delta at e^{-\delta t} + 1$$

$$y_2 = e^{-\delta t} [(y_2^0 - 1) + \delta (y_1^0 - 1)t] + 1$$

if $V_1 > V_2$

Appendix G

$V = 8 \text{ SCFM}$
 He

Overall Balance

at steady state

therefore,

$$\dot{n}_{\text{He}} + \dot{n}_{\text{H}_2} = \dot{n}_{\text{Ex}}$$

H₂ rate:

High Nominal: (peak rate) $1.9 \times 10^{-3} \text{ g/sec}$

Bounding: $2.4 \times 10^{-3} \text{ g/sec}$

Hydrogen Balance Around the MCOin: $\dot{n}_{H_2}$ out: $y \dot{n}_{ex}$ Accum: $\frac{d(yn)}{dt}$

$$n = \frac{PV}{RT}$$

$$y \frac{d\dot{n}}{dt} + n \frac{dy}{dt} = \dot{n}_{H_2} - y \dot{n}_{ex}$$

$$n \frac{dy}{dt} + y \dot{n}_{ex} - \dot{n}_{H_2} = 0$$

Can easily solve as previous problems with Integration factor.

$$\frac{\partial M}{\partial y} = \dot{n}_{ex} \quad \frac{\partial N}{\partial t} = 0$$

$$\frac{d\mu}{dt} = \left[\frac{\dot{n}_{ex}}{n} \right] \mu$$

$$\frac{d\mu}{\mu} = \frac{\dot{n}_{ex}}{n} dt$$

$$\therefore \ln \mu = \frac{\dot{n}_{ex} t}{n}$$

$$\mu = e^{\frac{\dot{n}_{ex} t}{n}}$$

Multiplying all terms by μ

$$n e^{\frac{\dot{n}_{ex} t}{n}} \frac{dy}{dt} + y \dot{n}_{ex} e^{\frac{\dot{n}_{ex} t}{n}} - \dot{n}_{H_2} e^{\frac{\dot{n}_{ex} t}{n}} = 0$$

checking "exactness"

$$\frac{\partial M^*}{\partial y} = \dot{n}_{ex} e^{\frac{\dot{n}_{ex} t}{n}}$$

$$\frac{\partial N^*}{\partial t} = \frac{\dot{n}_{ex}}{n} e^{\frac{\dot{n}_{ex} t}{n}}$$

exact
G-3

Therefore, there exists ψ such that

$$\frac{\partial \psi}{\partial t} = y \dot{n}_{ex} e^{\dot{n}_{ex} t / n} - \dot{n}_{ex} e^{\dot{n}_{ex} t / n} = e^{\dot{n}_{ex} t / n} [y \dot{n}_{ex} - \dot{n}_{ex}]$$

$$\psi = \frac{(y \dot{n}_{ex} - \dot{n}_{ex})}{\dot{n}_{ex} / n} e^{\dot{n}_{ex} t / n} + h(y) = C$$

$$\psi = \frac{n(y \dot{n}_{ex} - \dot{n}_{ex})}{\dot{n}_{ex}} e^{\dot{n}_{ex} t / n} + h(y)$$

$$\psi = (ny - n \frac{\dot{n}_{ex}}{\dot{n}_{ex}}) e^{\dot{n}_{ex} t / n} + h(y) = C$$

$$\frac{\partial \psi}{\partial y} = ne^{\dot{n}_{ex} t / n} + h'(y)$$

Setting equal to $\frac{\partial \psi}{\partial y} = ne^{\dot{n}_{ex} t / n}$

$$h'(y) = 0 \text{ and } h(y) = 0$$

Substituting into general sol'n:

$$(ny - n \frac{\dot{n}_{ex}}{\dot{n}_{ex}}) e^{\dot{n}_{ex} t / n} = C$$

and solving for C, e initial conditions $t=0$

$$C = ny_0 - n \frac{\dot{n}_{ex}}{\dot{n}_{ex}} \quad y = y_0$$

Therefore, solution is:

$$(ny - n \frac{\dot{n}_{ex}}{\dot{n}_{ex}}) e^{\dot{n}_{ex} t / n} = ny_0 - n \frac{\dot{n}_{ex}}{\dot{n}_{ex}}$$

and solving for y :

$$n(y - \frac{\dot{r}_{u2}}{\dot{r}_{e2}}) = e^{-\dot{r}_{e2}t/n} \left[y_0 - \frac{\dot{r}_{u2}}{\dot{r}_{e2}} \right] n$$

$$y = e^{-\dot{r}_{e2}t/n} \left[y_0 - \frac{\dot{r}_{u2}}{\dot{r}_{e2}} \right] + \frac{\dot{r}_{u2}}{\dot{r}_{e2}}$$

22-141 50 SHEETS
22-142 100 SHEETS
22-143 200 SHEETS

Appendix H

Problem 8

$$V_{MCO} = 500 \text{ L} \\ \approx 18 \text{ ft}^3$$

H₂ Rates

$$\text{HN: } 1.9 \times 10^{-3} \text{ g/sec} \\ \text{B: } 2.9 \times 10^{-3} \text{ g/sec}$$

Overall Balance

$$\text{in: } \dot{n}_{He} + \dot{n}_{H_2}$$

$$\text{out: } \dot{n}_{ex}$$

note: $\dot{n}_{ex}$ not constant, decreases with decreasing pressure
however, $\dot{V}_{ex}$ assumed constant

$$\text{Accum: } \frac{dn}{dt}$$

$$\therefore \dot{n}_{ex} = \frac{\dot{V}_{ex} P}{RT} = \frac{\dot{V}_{ex} (n \frac{RT}{V_{MCO}})}{RT} = \frac{n \dot{V}_{ex}}{V_{MCO}}$$

Therefore,

$$\frac{dn}{dt} = \dot{n}_{He} + \dot{n}_{H_2} - \frac{n \dot{V}_{ex}}{V_{MCO}}$$

$$\text{or} \\ \frac{1}{N} \frac{dN}{dt} + \frac{N \dot{V}_{ex}}{V} - (\dot{n}_{He} + \dot{n}_{H_2}) = 0$$

need to solve for n , check exactness as in previous ode problems

$$\frac{\partial M}{\partial n} = \frac{\dot{V}_{ex}}{V}$$

$$\frac{\partial N}{\partial t} = 0$$

not exact
therefore, need Integration Factor

$$\frac{d\mu}{dt} = \left[\frac{\frac{\partial M}{\partial n} - \frac{\partial N}{\partial t}}{N} \right] \mu = \frac{\dot{V}_{ex}}{V} \mu$$

$$\frac{d\mu}{\mu} = \frac{\dot{V}_{ex}}{V} dt$$

$$\ln \mu = \frac{\dot{V}_{ex}}{V} t$$

$$\mu = e^{\frac{\dot{V}_{ex}}{V} t}$$

H-2

$$t + \tau = \frac{V}{\dot{V}_{ex}}$$

Multiplying all terms by the Integration Factor:

$$e^{\delta t} \frac{dn}{dt} + e^{\delta t} [\delta n - (\dot{n}_{H_2} + \dot{n}_{H_2})] = 0$$

checking "exactness", $\frac{\partial M^T}{\partial n} = \delta e^{\delta t}$ $\frac{\partial N}{\partial t} = \delta e^{\delta t}$ ✓ exact

Therefore, there exists ψ such that,

$$\frac{\partial \psi}{\partial t} = e^{\delta t} [\delta n - (\dot{n}_{H_2} + \dot{n}_{H_2})]$$

$$\psi = \frac{1}{\delta} e^{\delta t} [\delta n - (\dot{n}_{H_2} + \dot{n}_{H_2})] + h(n) = C$$

and $\frac{\partial \psi}{\partial n} = e^{\delta t} + h'(n)$

Setting equal to $\frac{\partial \psi}{\partial n} = e^{\delta t}$ $\therefore h'(n) = 0$
 $h(n) = 0$

$$\therefore \frac{1}{\delta} e^{\delta t} [\delta n - (\dot{n}_{H_2} + \dot{n}_{H_2})] = C$$

Solving for C, at initial conditions $t=0$
 $n=n^0$

$$C = \frac{1}{\delta} [\delta n^0 - (\dot{n}_{H_2} + \dot{n}_{H_2})]$$

$$= n^0 - \frac{(\dot{n}_{H_2} + \dot{n}_{H_2})}{\delta}$$

Therefore, the sol'n is:

$$\frac{1}{\delta} e^{\delta t} [\delta n - (\dot{n}_{H_2} + \dot{n}_{H_2})] = n^0 - \frac{(\dot{n}_{H_2} + \dot{n}_{H_2})}{\delta}$$

$$e^{\delta t} [\delta n - (\dot{n}_{H_2} + \dot{n}_{H_2})] = \underbrace{\delta n^0 - (\dot{n}_{H_2} + \dot{n}_{H_2})}_{\pi}$$

Solving for n,

$$\delta n - (\dot{n}_{H_2} + \dot{n}_{H_2}) = \pi e^{-\delta t}$$

$$\gamma n = \pi e^{-\gamma t} + (\dot{n}_{H_2} + \dot{n}_{H_2})$$

$$n = \frac{\pi}{\gamma} e^{-\gamma t} + \frac{(\dot{n}_{H_2} + \dot{n}_{H_2})}{\gamma}$$

or

$$n = \frac{(\gamma n^0 - (\dot{n}_{H_2} + \dot{n}_{H_2}))}{\gamma} e^{-\gamma t} + \frac{(\dot{n}_{H_2} + \dot{n}_{H_2})}{\gamma}$$

$$n = n^0 e^{-\gamma t} - \frac{(\dot{n}_{H_2} + \dot{n}_{H_2})}{\gamma} e^{-\gamma t} + \frac{(\dot{n}_{H_2} + \dot{n}_{H_2})}{\gamma}$$

$$\text{let } \beta = \frac{(\dot{n}_{H_2} + \dot{n}_{H_2})}{\gamma}$$

$$\gamma = \frac{V_{ex}}{V_{mco}}$$

$$n = n^0 e^{-\gamma t} - \beta e^{-\gamma t} + \beta$$

$$n = e^{-\gamma t} (n^0 - \beta) + \beta$$

$$\begin{aligned} \frac{dn}{dt} &= (n^0 - \beta)(-\gamma) e^{-\gamma t} \\ &= \gamma (\beta - n^0) e^{-\gamma t} \end{aligned}$$

Hydrogen Balance

in: $\dot{n}_{H_2}$ out: $\dot{n}_{ex} y$ Accum: $\frac{d(\gamma n)}{dt}$

$$\begin{aligned} \text{note: } \dot{n}_{ex} &= \gamma n && \text{from Overall Balance} \\ &= \gamma [e^{-\gamma t} (n^0 - \beta) + \beta] \end{aligned}$$

$$\therefore \frac{d(\gamma n)}{dt} = \dot{n}_{H_2} - \dot{n}_{ex} y = \dot{n}_{H_2} - \gamma n y$$

$$n \frac{dy}{dt} + y \frac{dn}{dt} = \dot{n}_{H_2} - \gamma y n$$

$$n \frac{dy}{dt} + y \gamma (\beta - n^0) e^{-\gamma t} = \dot{n}_{H_2} - \gamma y n$$

$$n \frac{dy}{dt} + y\delta(\beta - n^2)e^{-\delta t} + \delta y n - \dot{n} = 0$$

checking for exact eqn: $\frac{\partial M}{\partial y} = \delta(\beta - n^2)e^{-\delta t} + \delta n$

$$n = e^{-\delta t}(n^2 - \beta) + \beta$$

$$\frac{\partial N}{\partial t} = (n^2 - \beta)(-\delta)e^{-\delta t} = -\delta(n^2 - \beta)e^{-\delta t} = \delta(\beta - n^2)e^{-\delta t}$$

not exact, therefore, need Integration Factor,

$$\frac{d\mu}{dt} = \left[\frac{\frac{\partial M}{\partial y} - \frac{\partial N}{\partial t}}{N} \right] \mu = \left[\frac{\delta(\beta - n^2)e^{-\delta t} + \delta n - \delta(\beta - n^2)e^{-\delta t}}{n} \right] \mu = \delta \mu$$

$$\frac{d\mu}{\mu} = \delta dt$$

$$\ln \mu = \delta t$$

$$\mu = e^{\delta t}$$

Multiply all terms by Integration Factor, μ

$$e^{\delta t} n \frac{dy}{dt} + y\delta(\beta - n^2) + e^{\delta t} \delta n y - e^{\delta t} \dot{n} = 0$$

checking "exactness,"

$$\frac{\partial M^*}{\partial y} = \delta(\beta - n^2) + \delta n e^{\delta t} = \delta \beta e^{\delta t} -$$

$$e^{\delta t} n = e^{\delta t} (e^{-\delta t}(n^2 - \beta) + \beta) = (n^2 - \beta) + \beta e^{\delta t}$$

$$\frac{\partial N^*}{\partial t} = \delta \beta e^{\delta t} \quad \text{exact}$$

Simplifying $\frac{\partial M^*}{\partial y} = \delta(\beta - n^2) + \delta n e^{\delta t}$

$$\delta(\beta - n^2) + \delta(e^{-\delta t}(n^2 - \beta) + \beta)e^{\delta t}$$

$$= \delta(\beta - n^2) + \delta(n^2 - \beta) + \delta \beta e^{\delta t}$$

$$= \delta \beta - \delta n^2 + \delta n^2 - \delta \beta + \delta \beta e^{\delta t} = \delta \beta e^{\delta t}$$

Therefore, there exists ψ such that,

$$\frac{\partial \psi}{\partial t} = y(\beta - n^0) + e^{\sigma t} \sigma n y - e^{\sigma t} \dot{n}_{H_2}$$

$$\psi = y(\beta - n^0)t - \frac{\dot{n}_{H_2}}{\sigma} e^{\sigma t} + [\sigma y(n^0 - \beta)t + y\beta e^{\sigma t}] + h(y) = C$$

$$e^{\sigma t} \sigma n y = \sigma y e^{\sigma t} (e^{-\sigma t} (n^0 - \beta) + \beta)$$

$$= \sigma y (n^0 - \beta) + \sigma y \beta e^{\sigma t}$$

$$\psi = y\beta e^{\sigma t} - \frac{\dot{n}_{H_2}}{\sigma} e^{\sigma t} + h(y) = C$$

and

$$\frac{\partial \psi}{\partial y} = \beta e^{\sigma t} + h'(y)$$

Setting equal to $\frac{\partial \psi}{\partial y} = e^{\sigma t} n$

$$= (n^0 - \beta) + \beta e^{\sigma t}$$

$$\therefore h'(y) = n^0 - \beta$$

$$\text{and } h(y) = (n^0 - \beta)y$$

Substituting into general sol'n:

$$y\beta e^{\sigma t} - \frac{\dot{n}_{H_2}}{\sigma} e^{\sigma t} + (n^0 - \beta)y = C$$

Solving for C, c initial conditions $t=0$
 $y=y^0$

$$C = y_0 \beta - \frac{\dot{n}_{H_2}}{\sigma} + (n^0 - \beta)y_0$$

$$C = y_0 \beta - \frac{\dot{n}_{H_2}}{\sigma} + n^0 y_0 - \beta y_0$$

$$C = n^0 y_0 - \frac{\dot{n}_{H_2}}{\sigma}$$

Substituting into general sol'n:

$$y\beta e^{\delta t} - \frac{\dot{n}_{H_2}}{\delta} e^{\delta t} + (n^0 - \beta)y = n^0 y_0 - \frac{\dot{n}_{H_2}}{\delta}$$

and solving for y,

$$y(\beta e^{\delta t} + (n^0 - \beta)) = n^0 y_0 - \frac{\dot{n}_{H_2}}{\delta} + \frac{\dot{n}_{H_2}}{\delta} e^{\delta t}$$

$$y(\beta(e^{\delta t} - 1) + n^0) = \frac{\dot{n}_{H_2}}{\delta}(e^{\delta t} - 1) + n^0 y_0$$

$$\therefore y = \frac{\left[\frac{\dot{n}_{H_2}}{\delta}(e^{\delta t} - 1) + n^0 y_0 \right]}{\left[\beta(e^{\delta t} - 1) + n^0 \right]}$$

checking @ $t=0$

$$y = \frac{n^0 y_0}{n^0} = y_0 \quad \checkmark$$

Putting into $P = f(y)$

From Overall Balance,

$$n = (n^0 - \beta)e^{-\delta t} + \beta$$

$$\frac{PV_{mco}}{RT} = \left(\frac{P^0 V}{RT} - \beta \right) e^{-\delta t} + \beta$$

$$\therefore P = \frac{RT}{V_{mco}} \left[\left(\frac{P^0 V}{RT} - \beta \right) e^{-\delta t} + \beta \right]$$

$$\delta = \frac{\dot{V}_{ex}}{V_{mco}}$$

$$\beta = \frac{(\dot{n}_{H_2} + \dot{n}_{H_2})}{\delta}$$

$$n^0 = \frac{P^0 V_{mco}}{RT}$$

$$n = \frac{PV_{mco}}{RT} \quad n^0 = \frac{P^0 V_{mco}}{RT}$$

$$V_{total} = (V_{He} \text{ cscfm}) t \text{ (sec)}$$

$$P = \frac{nRT}{V_{mco}}$$

Problem 8

- if vacuum line breaks - no vacuum

Overall Balance

in: $\dot{n}_{He} + \dot{n}_m$

out: $\dot{n}_{ex}$

Accum: $\frac{dn}{dt} = 0$

$\therefore \dot{n}_m + \dot{n}_{He} = \dot{n}_{ex}$

Hydrogen Balance

in: $\dot{n}_{H_2}$

out: $\dot{n}_{ex} y$

Accum: $\frac{d(ny)}{dt}$

$n \frac{dy}{dt} + y \frac{dn}{dt} \stackrel{0 \text{ ss}}{=} \dot{n}_{H_2} - \dot{n}_{ex} y$

$\therefore n \frac{dy}{dt} + \dot{n}_{ex} y - \dot{n}_{H_2} = 0$

need Integrating Factor,

$\frac{\partial M}{\partial y} = \dot{n}_{ex}$

$\frac{dM}{dt} = \frac{\dot{n}_{ex}}{n} M$

$\ln \frac{M}{M_0} = \frac{\dot{n}_{ex}}{n} dt$

let $t = \frac{\dot{n}_{ex}}{n}$

$M = e^{rt}$

Multiplying all terms by μ ,

$$\mu e^{rt} \frac{dy}{dt} + e^{rt} (\dot{n}_{ex} y - \dot{n}_{in}) = 0$$

checking "exactness"

$$\frac{\partial M^S}{\partial y} = \dot{n}_{ex} e^{rt} -$$

$$\frac{\partial M^S}{\partial t} = \mu e^{rt} = \dot{n}_{ex} e^{rt} -$$

Therefore, there exists ψ such that,

$$\frac{\partial \psi}{\partial t} = e^{rt} (\dot{n}_{ex} y - \dot{n}_{in})$$

$$\psi = \frac{(\dot{n}_{ex} y - \dot{n}_{in})}{r} e^{rt} + h(y) = C$$

General Soln

$$\psi = \frac{\eta}{\dot{n}_{ex}} (\dot{n}_{ex} y - \dot{n}_{in}) e^{rt} + h(y)$$

and

$$\frac{\partial \psi}{\partial y} = \eta e^{rt} + h'(y)$$

setting equal to $\frac{\partial \psi}{\partial y} = \eta e^{rt}$

$$\therefore h'(y) = 0 \text{ and } h(y) = 0$$

Substituting into general solution

$$\psi = \frac{\eta}{\dot{n}_{ex}} (\dot{n}_{ex} y - \dot{n}_{in}) e^{rt} = C$$

and solving for C , @ initial conditions $t=0$
 $y=y_0$

$$C = \frac{\eta}{\dot{n}_{ex}} (\dot{n}_{ex} y_0 - \dot{n}_{in})$$

and substituting into general sol'n:

$$\frac{1}{\dot{n}_{ex}} (\dot{n}_{ex} y - \dot{n}_{H_2}) e^{\delta t} = \frac{1}{\dot{n}_{ex}} (\dot{n}_{ex} y_0 - \dot{n}_{H_2})$$

and solving for y:

$$\dot{n}_{ex} y - \dot{n}_{H_2} = e^{-\delta t} (\dot{n}_{ex} y_0 - \dot{n}_{H_2})$$

$$\dot{n}_{ex} y = e^{-\delta t} (\dot{n}_{ex} y_0 - \dot{n}_{H_2}) + \dot{n}_{H_2}$$

$$y = e^{-\delta t} \left(y_0 - \frac{\dot{n}_{H_2}}{\dot{n}_{ex}} \right) + \frac{\dot{n}_{H_2}}{\dot{n}_{ex}}$$

$$\text{where } \dot{n}_{ex} = \dot{n}_{H_2} + \dot{n}_{H_2O}$$

or solving for P,

$$e^{-\delta t} = \frac{(\dot{n}_{ex} y_0 - \dot{n}_{H_2})}{(\dot{n}_{ex} y - \dot{n}_{H_2})} = \pi$$

$$\delta t = \ln \pi$$

$$\delta = \frac{\dot{n}_{ex}}{n}$$

$$\frac{\dot{n}_{ex} t}{n} = \ln \pi$$

$$n = \frac{P V_{mco}}{RT}$$

$$\frac{\dot{n}_{ex} t}{\ln \pi} = n = \frac{P V_{mco}}{RT}$$

or

$$P = \frac{RT}{V_{mco}} \frac{\dot{n}_{ex} t}{\ln \pi}$$

Appendix I

PROBLEM 9

H₂ RateHigh Nominal: 1.9×10^{-3} g/secBounding: 2.4×10^{-3} g/sec

This problem is set up and solved as in Problem 8.

where:

$$y = \frac{\left[\frac{\dot{n}_{H_2}}{r} (e^{rt} - 1) + n_0^y \right]}{\left[\beta (e^{rt} - 1) + n^0 \right]}$$

and

$$\gamma = \frac{\dot{V}_{ex}}{V_{MCD}}$$

$$\beta = \frac{(\dot{n}_{He} + \dot{n}_{H_2})}{\gamma}$$

$$n^0 = \frac{P^0 V_{MCD}}{RT}$$

$$P = \frac{RT}{V_{MCD}} \left[\left(\frac{P^0 V}{RT} - \beta \right) e^{-\gamma t} + \beta \right]$$

 $P^0 = 0.5 \text{ atm}$ to $P = 140 \text{ torr}$ and below

Appendix J

Prob. 10

$$V_0 = 0.56 \text{ ft}^3$$

$$T = 50^\circ\text{C} = 323 \text{ K}$$

$$\frac{dV}{dt} = 6 \frac{\text{gal}}{\text{min}}$$

Overall Balance

$$\text{in: } \dot{n}_{\text{H}_2} + \dot{n}_{\text{air}}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{dn}{dt}$$

assume
T, P constant

$$\frac{dn}{dt} = \dot{n}_{\text{H}_2} + \dot{n}_{\text{air}} = \frac{P}{RT} \frac{dV}{dt} = \alpha$$

$$n - n_0 = \alpha t$$

$$n = \alpha t + n_0$$

Air Balance

$$\text{in: } \dot{n}_{\text{air}}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{d(ny)}{dt}$$

$$n \frac{dy}{dt} + y \frac{dn}{dt} = \dot{n}_{\text{air}}$$

$$n \frac{dy}{dt} + 2y - \dot{n}_{\text{air}} = 0$$

checking "exactness"

$$\frac{\partial M}{\partial y} = 2$$

$$\frac{\partial N}{\partial t} = 2$$

— exact

Therefore, there exists Ψ such that:

$$\frac{\partial \Psi}{\partial t} = \alpha y - \dot{n}_{21r}$$

$$\Psi = (\alpha y - \dot{n}_{21r})t + h(y) = C \quad \leftarrow \text{General Sol'n}$$

$$\frac{\partial \Psi}{\partial y} = \alpha t + h'(y)$$

Setting equal to $\frac{\partial \Psi}{\partial y} = \alpha t + n_0$

$$\therefore h'(y) = n_0 \quad \therefore h(y) = n_0 y$$

$$\therefore (\alpha y - \dot{n}_{21r})t + n_0 y = C$$

Solving for C, at $t=0$ $y=y_0$

$$C = n_0 y_0$$

$$(\alpha y - \dot{n}_{21r})t + n_0 y = n_0 y_0$$

and solving for y,

$$\alpha y t - \dot{n}_{21r} t + n_0 y = n_0 y_0$$

$$y(\alpha t + n_0) = \dot{n}_{21r} t + n_0 y_0$$

$$\therefore y_{21r} = \frac{(\dot{n}_{21r} t + n_0 y_0)}{(\alpha t + n_0)}$$

$$\therefore y_{02} = 0.21 * y_{21r}$$

H₂ Balancein: $\dot{n}_{H_2}$

out: 0

Accum: $\frac{d(ny)}{dt}$

$$n \frac{dy}{dt} + y \frac{dn}{dt} = \dot{n}_{H_2}$$

$$n \frac{dy}{dt} + dy - \dot{n}_{H_2} = 0 \quad \text{exact}$$

Therefore, there exists Ψ such that

$$\frac{\partial \Psi}{\partial t} = dy - \dot{n}_{H_2}$$

$$\Psi = (dy - \dot{n}_{H_2})t + h(y) = C \quad \text{General Sol'n}$$

and

$$\frac{\partial \Psi}{\partial y} = dt + h'(y)$$

Setting equal to $\frac{\partial \Psi}{\partial y} = dt + n_0$

$$\therefore h'(y) = n_0 \quad \text{and} \quad h(y) = n_0 y$$

$$\therefore (dy - \dot{n}_{H_2})t + n_0 y = C$$

$$C \quad t=0 \quad y=y_0$$

$$C = n_0 y_0$$

$$\therefore (dy - \dot{n}_{H_2})t + n_0 y = n_0 y_0$$

$$dyt - \dot{n}_{H_2}t + n_0 y = n_0 y_0$$

$$y(dt + n_0) = \dot{n}_{H_2}t + n_0 y_0 \quad \xrightarrow{\text{I-4}} \quad y_{H_2} = \frac{(\dot{n}_{H_2}t + n_0 y_0)}{(dt + n_0)}$$

Appendix K

Prob 11

Overall Balance

$$\text{in: } \dot{n}_{\text{air}} + \dot{n}_{\text{H}_2} = 2$$

$$\text{out: } \dot{n}_{\text{ex}}$$

$$\text{Accum: } \frac{dn}{dt}$$

$$\frac{dn}{dt} = \frac{V}{RT} \frac{dP}{dt} = 2 - \dot{n}_{\text{ex}}$$

$$P(\text{psia}) = a' + b' \dot{n}_{\text{ex}} + c' \dot{n}_{\text{ex}}^2$$

$$\frac{dP}{dt} = \frac{dP}{d\dot{n}_{\text{ex}}} \frac{d\dot{n}_{\text{ex}}}{dt}$$

$$\frac{dP}{d\dot{n}_{\text{ex}}} = b' + 2c' \dot{n}_{\text{ex}} \quad \leftarrow \text{see pg 4}$$

Solving for $\dot{n}_{\text{ex}}$:

$$\frac{V}{RT} \frac{dP}{dt} = 2 - \dot{n}_{\text{ex}}$$

$$\frac{V}{RT} \frac{dP}{d\dot{n}_{\text{ex}}} \frac{d\dot{n}_{\text{ex}}}{dt} = 2 - \dot{n}_{\text{ex}}$$

$$\frac{V}{RT} (b' + 2c' \dot{n}_{\text{ex}}) \frac{d\dot{n}_{\text{ex}}}{dt} = 2 - \dot{n}_{\text{ex}}$$

$$\frac{d\dot{n}_{\text{ex}}}{dt} = \frac{(2 - \dot{n}_{\text{ex}})}{(b' + 2c' \dot{n}_{\text{ex}})} \frac{RT}{V}$$

$$2 = \dot{n}_{\text{air}} + \dot{n}_{\text{H}_2}$$

$$\dot{n}_{\text{ex}}^0 = 0.05512 \quad \text{see [12]}$$

$$\frac{dn}{dt} = 2 - \dot{n}_{\text{ex}}$$

$$\frac{dy_{\text{air}}}{dt} = \frac{1}{n} \left[\dot{n}_{\text{air}} - \dot{n}_{\text{ex}} y_{\text{air}} - y_{\text{air}} \frac{dn}{dt} \right] \quad \leftarrow \text{from pg 3}$$

$$\frac{dy_{\text{H}_2}}{dt} = \frac{1}{n} \left[\dot{n}_{\text{H}_2} - \dot{n}_{\text{ex}} y_{\text{H}_2} - y_{\text{H}_2} \frac{dn}{dt} \right] \quad \leftarrow \text{from pg 3}$$

K-2

Initial values

$$\dot{n}_{\text{ex}}^0 = 18.14 \text{ g mol/min}$$

$$n^0 = \frac{P^0 V}{RT}$$

$$y_{\text{air}}^0 = 0$$

$$y_{\text{H}_2}^0 = 0.01$$

$$V = 18 \text{ ft}^3$$

$$\dot{n}_{\text{H}_2} = 0.072 \frac{\text{g mol}}{\text{min}} \quad \leftarrow \text{see pg 4}$$

$$\dot{n}_{\text{air}} = \frac{P \dot{V}_{\text{air}}}{RT}$$

$$P = 14.696 \text{ psia}$$

$$T = 70^\circ \text{F} = 21^\circ \text{C} = 294$$

$$b' = 1.1554 \frac{\text{psia} \cdot \text{min}}{\text{g mol}}$$

$$c' = -0.0217 \frac{\text{psia} \cdot \text{min}^2}{\text{g mol}^2}$$

$$n^0 = \frac{P^0 V}{RT}$$

Air Balancein: $\dot{n}_{air}$ out: $\dot{n}_{ex} y_{air}$ Accum: $\frac{d(ny)}{dt}$

$$n \frac{dy_{air}}{dt} + y_{air} \frac{dn}{dt} = \dot{n}_{air} - \dot{n}_{ex} y_{air}$$

$$n \frac{dy_{air}}{dt} = \dot{n}_{air} - \dot{n}_{ex} y_{air} - y_{air} \frac{dn}{dt}$$

$$\frac{dy_{air}}{dt} = \frac{1}{n} \left[\dot{n}_{air} - \dot{n}_{ex} y - y \frac{dn}{dt} \right]$$

H₂ Balancein: $\dot{n}_{H_2}$ out: $\dot{n}_{ex} y_{H_2}$ Accum: $\frac{d(ny_{H_2})}{dt}$

$$n \frac{dy_{H_2}}{dt} + y_{H_2} \frac{dn}{dt} = \dot{n}_{H_2} - \dot{n}_{ex} y_{H_2}$$

$$n \frac{dy_{H_2}}{dt} = \dot{n}_{H_2} - \dot{n}_{ex} y_{H_2} - y_{H_2} \frac{dn}{dt}$$

$$\frac{dy_{H_2}}{dt} = \frac{1}{n} \left[\dot{n}_{H_2} - \dot{n}_{ex} y_{H_2} - y_{H_2} \frac{dn}{dt} \right]$$

$$P = 1.7858 + 2.9729 \dot{V} - 0.0706 \dot{V}^2$$

$$P = 14.696 \text{ psia}$$

$$R = 0.04259 \frac{\text{ft}^3}{\text{gmol}}$$

$$T = 273 \text{ K}$$

$$\beta = \frac{RT}{P} = 0.7912 \frac{\text{ft}^3}{\text{gmol}}$$

$$\beta \text{ c.s.c.}$$

$$PV = nRT$$

$$\dot{V} = \frac{\dot{n}RT}{P}$$

$$\dot{n} \left(\frac{RT}{P} \right) = \dot{n} \beta$$

$$\frac{\text{in Hg} \cdot \text{min}}{\text{ft}^3}$$

$$\frac{\text{in Hg} \cdot \text{min}^2}{\text{ft}^6}$$

$$P_{\text{in Hg}} = 1.7858 + 2.9729 \beta \dot{n} - 0.0706 (\dot{n} \beta)^2$$

$$P_{\text{in Hg}} = 1.7858 + 2.3522 \dot{n}_{\text{ex}} - 0.0442 \dot{n}_{\text{ex}}^2$$

$$0.4912$$

$$P_{\text{in Hg}} \times \frac{(14.696 \text{ psia})}{29.92 \text{ in Hg}} =$$

$$P(\text{psia}) = 0.4912 [1.7858 + 2.3522 \dot{n}_{\text{ex}} - 0.0442 \dot{n}_{\text{ex}}^2]$$

$$P_{\text{psia}} = 0.8772 + 1.1554 \dot{n}_{\text{ex}} - 0.0217 \dot{n}_{\text{ex}}^2$$

or

$$P_{\text{psia}} = a_0' \dot{n}_{\text{ex}}^2 + a_1' \dot{n}_{\text{ex}} + a_2'$$

$$a_0' = -0.0217 \frac{\text{psia} \cdot \text{min}^2}{\text{gmol}^2}$$

$$a_1' = 1.1554 \frac{\text{psia} \cdot \text{min}}{\text{gmol}}$$

$$a_2' = 0.8772 \text{ psia}$$

To find $\dot{n}_{ex}^0$:

$$c \quad P = P^0 = 14,696 \text{ psia}$$

from $P = f(\dot{n}_{ex})$ to form quadratic eqn and solve roots,

$$14,696 = -0.0217 \dot{n}_{ex}^2 + 1,1554 \dot{n}_{ex} + 0,8772$$

$$-0.0217 \dot{n}_{ex}^2 + 1,1554 \dot{n}_{ex} - 13,819 = 0$$

Solving for roots,

$$\text{where: } a = -0,0217$$

$$\dot{n}_{ex} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$b = 1,1554$$

$$c = -13,819$$

$$\text{root 1} = 35,10$$

$$\text{root 2} = 18,14 \quad \checkmark$$

2" ϕ 60 psigT = ⁸⁰~~90~~°FEductor Plot

<u>Suction Pressure (in H_2O)</u>	<u>SCFM AIR</u>	<u>(SCFM)</u>
(latm) 29.92	$3.5 \times 4 = 14$	
27	$3.0 \times 4 = 12$	
24	$2.5 \times 4 = 10$	
21	$2.0 \times 4 = 8$	
17.5	$1.5 \times 4 = 6$	
13	$1.0 \times 4 = 4$	5
7	$0.5 \times 4 = 2$	
1.8	$0 = 0$	

Fit 2ND Order polynomial- least squares fit
(MATLAB)- 2nd order fit

$$P = a_0 + a_1 \dot{V} + a_2 \dot{V}^2$$

$$a_0 = 1.7858$$

$$a_1 = 2.9729$$

$$a_2 = -0.0706$$

Appendix L

Prob 12

$$P_{final} = 4 \text{ psig}$$

Overall Balance

$$\text{in: } \dot{n}_{He} + \dot{n}_{H2}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{dn}{dt}$$

$$\frac{dn}{dt} = \dot{n}_{He} + \dot{n}_{H2} = \alpha$$

$$n = \alpha t + n_0$$

Air Balance

$$\text{in: } 0$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{d(ny)}{dt}$$

$$n \frac{dy}{dt} + y \frac{dn}{dt} = 0$$

$$n \frac{dy}{dt} + \alpha y = 0$$

exact

Therefore, there exists γ such that:

$$\frac{\partial \gamma}{\partial t} = \alpha y$$

$$\gamma = \alpha y t + h(y) = C \quad \leftarrow \text{General Soln}$$

and

$$\frac{\partial \Psi}{\partial y} = \alpha t + h'(y)$$

Setting equal to $\frac{\partial \Psi}{\partial y} = n = \alpha t + n_0$

$$\therefore h'(y) = n_0 \quad \text{and} \quad h(y) = n_0 y$$

substituting back into General Sol'n:

$$\alpha y t + n_0 y = C$$

and solving for C, C at $t=0$ $y=y_0$

$$C = n_0 y_0$$

$$\therefore \alpha y t + n_0 y = n_0 y_0$$

and solving for y:

$$y(\alpha t + n_0) = n_0 y_0$$

$$y_{01} = \frac{n_0 y_0}{(\alpha t + n_0)}$$

$$\text{and } y_{02} = 0.21 y_{01}$$

M₂ Balance

in: $\dot{m}_2$

out: 0

Accum: $\frac{d(ny)}{dt}$

$$n \frac{dy}{dt} + y \frac{dn}{dt} = \dot{m}_2$$

$$n \frac{dy}{dt} + \alpha y - \dot{n}_{H_2} = 0 \quad \text{exact}$$

∴ There exists ψ such that:

$$\frac{\partial \psi}{\partial t} = \alpha y - \dot{n}_{H_2}$$

$$\psi = \alpha y t - \dot{n}_{H_2} t + h(y) = C \quad \leftarrow \text{General Sol'n}$$

and

$$\frac{\partial \psi}{\partial y} = \alpha t + h'(y)$$

$$\text{Setting equal to } \frac{\partial \psi}{\partial y} = n = \alpha t + n_0$$

$$\therefore h'(y) = n_0 \quad \text{and} \quad h(y) = n_0 y$$

$$\alpha y t - \dot{n}_{H_2} t + n_0 y = C$$

and solving for C, at $t=0$ $y=y_0$

$$C = n_0 y_0$$

$$\therefore \alpha y t - \dot{n}_{H_2} t + n_0 y = n_0 y_0$$

and solving for y,

$$y(\alpha t + n_0) = n_0 y_0 + \dot{n}_{H_2} t$$

$$y_{H_2} = \frac{(\dot{n}_{H_2} t + n_0 y_0)}{(\alpha t + n_0)}$$

Steady StateOverall Balance

$$\text{in: } \dot{n}_{\text{He}} + \dot{n}_{\text{H}_2} = 2$$

$$\text{out: } \dot{n}_{\text{ex}}$$

$$\text{Accum: } \frac{dn}{dt} = 0$$

$$\therefore \dot{n}_{\text{ex}} = 2$$

Air Balance

$$\text{in: } 0$$

$$\text{out: } \dot{n}_{\text{ex}} y_{\text{air}}$$

$$\text{Accum: } \frac{d(n y_{\text{air}})}{dt}$$

$$n \frac{dy_{\text{air}}}{dt} + y_{\text{air}} \frac{dn}{dt} \overset{0}{=} 0 - \dot{n}_{\text{ex}} y_{\text{air}}$$

$$n \frac{dy_{\text{air}}}{dt} + \dot{n}_{\text{ex}} y_{\text{air}} = 0$$

$$n = \frac{PV}{RT}$$

$$\frac{dy_{\text{air}}}{dt} = -\frac{\dot{n}_{\text{ex}} y_{\text{air}}}{n} = -\phi y_{\text{air}}$$

$$\text{let } \phi = \frac{\dot{n}_{\text{ex}}}{n} = \frac{\alpha}{n}$$

$$\frac{dy_{\text{air}}}{y_{\text{air}}} = -\phi dt$$

$$\ln \frac{y_{\text{air}}}{y_{\text{air}}^0} = -\phi t$$

$$\therefore y_{\text{air}} = y_{\text{air}}^0 e^{-\phi t}$$

L-5

$$\therefore y_{\text{O}_2} = 0.21 y_{\text{air}}$$

H₂ Balancein: $\dot{n}_{H_2}$ out: $\dot{n}_{ex} y_{H_2}$ Accum: $\frac{d(n y_{H_2})}{dt}$

$$n \frac{dy_{H_2}}{dt} + y_{H_2} \frac{dn}{dt} = \dot{n}_{H_2} - \dot{n}_{ex} y_{H_2}$$

$$n \frac{dy_{H_2}}{dt} + \dot{n}_{ex} y_{H_2} - \dot{n}_{H_2} = 0$$

need Integration Factor, μ

$$\frac{\partial M}{\partial y_{H_2}} = \dot{n}_{ex}$$

$$\frac{d\mu}{dt} = \frac{\dot{n}_{ex}}{n} \mu = \phi \mu$$

$$\ln \mu = \phi t$$

$$\mu = e^{\phi t}$$

Multiplying all terms by μ ,

$$n e^{\phi t} \frac{dy_{H_2}}{dt} + \dot{n}_{ex} y_{H_2} e^{\phi t} - \dot{n}_{H_2} e^{\phi t} = 0$$

Therefore,

$$\frac{\partial \Psi}{\partial t} = \dot{n}_{ex} y_{H_2} e^{\phi t} - \dot{n}_{H_2} e^{\phi t}$$

$$\Psi = \frac{\dot{n}_{ex} y_{H_2} e^{\phi t}}{\phi} - \frac{\dot{n}_{H_2} e^{\phi t}}{\phi} + h(y_{H_2}) = C$$

$$\Psi = n y_{H_2} e^{\phi t} - \frac{\dot{n}_{H_2} e^{\phi t}}{\phi} + h(y_{H_2}) = C$$

General Sol'n

$$\frac{\partial \Psi}{\partial y_{H_2}} = n e^{\phi t} + h'(y_{H_2})$$

Setting equal to $\frac{\partial \Psi}{\partial y_{H_2}} = n e^{\phi t}$

$$\therefore h'(y_{H_2}) = 0 \text{ and } h(y_{H_2}) = 0$$

$$\therefore n y_{H_2} e^{\phi t} - \frac{\dot{n}_{H_2}}{\phi} e^{\phi t} = C$$

Solving for C, at $t=0$ $y_{H_2} = y_{H_2}^0$

$$C = n y_{H_2}^0 - \frac{\dot{n}_{H_2}}{\phi}$$

$$\therefore n y_{H_2} e^{\phi t} - \frac{\dot{n}_{H_2}}{\phi} e^{\phi t} = n y_{H_2}^0 - \frac{\dot{n}_{H_2}}{\phi}$$

$$\text{or } n y_{H_2} e^{\phi t} - \frac{\dot{n}_{H_2}}{\dot{n}_{Ex}} e^{\phi t} = n y_{H_2}^0 - \frac{\dot{n}_{H_2}}{\dot{n}_{Ex}}$$

Solving for y_{H_2} :

$$y_{H_2} = \left(y_{H_2}^0 - \frac{\dot{n}_{H_2}}{\dot{n}_{Ex}} \right) e^{-\phi t} + \frac{\dot{n}_{H_2}}{\dot{n}_{Ex}}$$

$$L = \dot{n}_{Ex}$$

Appendix M

Prob. 13

Bounding mass flow rate:

Assume 155°F
(H₂)

$$\dot{n}_{H_2} = \dot{V} \frac{\rho}{MW} = \frac{P \dot{V}}{RT} = \frac{(1 \text{ atm})(10 \text{ ft}^3/\text{min})(2 \frac{\text{lb}_m}{\text{lb}_m \text{ mol}})}{(0.729 \frac{\text{ft}^3 \cdot \text{atm}}{\text{lb}_m \cdot ^\circ \text{R}})(491.4^\circ \text{R})}$$

limit $\rightarrow \dot{V} = 10 \text{ SCFM}$

273 K

$$\therefore \dot{n} = 0.0558 \frac{\text{lb}_m \text{ H}_2}{\text{min}}$$

$$\dot{n}_{H_2} (\text{mol/min}) = 0.0558 \frac{\text{lb}_m}{\text{min}} \times \frac{1 \text{ lb}_m}{2 \text{ lb}_m} \times \frac{4.94}{1 \text{ lb}_m} = 12.67 \text{ mol H}_2/\text{min}$$

Since the pressure ratio, $\frac{P_0}{P_1} \approx 11.2$ is well over 11:1

$$P_0 = 164.7 \text{ psia} (150 \text{ psig})$$

$$P_1 = 14.7 \text{ psia} (1 \text{ atm})$$

critical flow $\hookrightarrow P_1 = 97 \text{ psia}$
see pg 5use $G_{H_2}^*$ (from Perry's) $\therefore$ Eqn (3.27) $\leftarrow$ (Levenspiel 1984) — Also, Perry's 6th ed Eqn 5-21 pg 5-14

$$G_{H_2}^* = C P_0 \left[\frac{g_c (MW) k}{RT_0} \left(\frac{2}{1+k} \right)^{(k+1)/(k-1)} \right]^{1/2}$$

$$\text{For H}_2, k = 1.4 \quad (k = \frac{C_p}{C_v})$$

$$C \approx 0.75 \quad (\text{see Perry's 6th ed. pg 5-16})$$

$$P_0 = 164.7 \text{ psia}$$

$$R^* = 0.729 \frac{\text{ft}^3 \cdot \text{atm}}{\text{lb}_m \cdot ^\circ \text{R}}$$

$$g_c^* = 32.16 \frac{\text{lb}_m \cdot \text{ft}}{\text{lb}_f \cdot \text{sec}^2}$$

$$T_0 = 50^\circ \text{C} = 582^\circ \text{R}$$

$$MW_{H_2} = \frac{2 \text{ lb}_m}{\text{lb}_m \text{ mol}}$$

units correct

$$\rightarrow R' = 0.729 \frac{\text{ft}^3 \cdot \text{atm}}{\text{lb}_m \cdot ^\circ \text{R}} \times \frac{14.696 \text{ lb}_f}{1 \text{ atm} \cdot \text{in}^2} \times \frac{144 \text{ in}^2}{\text{ft}^2} = 1593$$

$$R' = R \times 2116.2 = 1593 \frac{\text{ft} \cdot \text{lb}_f}{\text{lb}_m \cdot ^\circ \text{R}}$$

$$\rightarrow g_c' = 32.16 \frac{\text{lb}_m \cdot \text{ft}}{\text{lb}_f \cdot \text{sec}^2} \times \left(\frac{60 \text{ sec}}{1 \text{ min}} \right)^2 = 115,776 \frac{\text{lb}_m \cdot \text{ft}}{\text{lb}_f \cdot \text{min}^2}$$

$$g_c' = g_c \times 3600 =$$

$$\text{let } \phi = k \left[\frac{z}{(1+k)} \right]^{\frac{(k+1)}{(k-1)}}$$

$$G_{N_2}^* = P_0 \left[\frac{g_c' (MW) \phi}{R' T_0} \right]^{1/2} \equiv \frac{15 \text{ m}}{\text{in}^2 \cdot \text{min}}$$

let A = cross-sectional area of orifice (in^2)

$$\therefore G_{N_2}^* A_{cs} = \dot{m}$$

$$A_{cs} = \frac{\dot{m}}{G_{N_2}^*} = \frac{\pi D^2}{4}$$

$$\therefore D = \sqrt{\frac{4 \cdot \dot{m}}{\pi G_{N_2}^*}} \quad (\text{in})$$

for H_2 , $k=1.4$
 $k = C_p / C_v$

$$r_c = \frac{P_2}{P_1}$$

$$r_c = \left(\frac{z}{(k+1)} \right)^{k/(k-1)}$$

→ Eqn (5-19),
 Perry's 6th
 pg 5-14

for H_2 ,

$$r_c = 0.528$$

$$\therefore P_1 = 150 \text{ psia} = 164.7 \text{ psia}$$

$$P_2 \text{ will not fall below } P_1 r_c \text{ or } (164.7 \text{ psia})(0.528) = 86.96 \approx 87 \text{ psia}$$

Appendix N

rob. 14

Overall Balance

in: $\dot{n}_{H_2}$

out: $\dot{n}_{E_2}$

Accum: $\frac{dn}{dt}$

$$\dot{n}_{E_2} = \frac{P \dot{V}_{E_2}}{RT} = n \left(\frac{\dot{V}_{E_2}}{V} \right) \quad \left(\frac{P}{RT} = \frac{n}{V} \right)$$

$$\frac{dn}{dt} = \dot{n}_{H_2} - n \left(\frac{\dot{V}_{E_2}}{V} \right)$$

$$\text{let } k = \frac{\dot{V}_{E_2}}{V}$$

$$\therefore \frac{dn}{dt} + kn - \dot{n}_{H_2} = 0$$

Need Integration Factor, μ

$$\frac{\partial \mu}{\partial n} = k$$

$$\frac{d\mu}{dt} = k\mu$$

$$\ln \mu = kt$$

$$\therefore \mu = e^{kt}$$

Multiplying all terms by μ ,

$$e^{kt} \frac{dn}{dt} + k n e^{kt} - e^{kt} \dot{n}_{H_2} = 0$$

Therefore, there exists ψ such:

$$\frac{\partial \psi}{\partial t} = k n e^{kt} - e^{kt} \dot{n}_{H_2}$$

$$\psi = n e^{kt} - \frac{\dot{n}_{H_2}}{k} e^{kt} + h(n) = C \quad \text{General Sol'n}$$

and

$$\frac{\partial \Psi}{\partial n} = e^{kt} + h'(n)$$

Setting equal to $\frac{\partial \Psi}{\partial n} = e^{kt}$

$$\therefore h'(n) = 0 \text{ and } h(n) = 0$$

$$\therefore ne^{kt} - \frac{\dot{n}_{H_2}}{k} e^{kt} = C$$

$$C \quad t=0 \quad n=n_0$$

$$\therefore C = n_0 - \frac{\dot{n}_{H_2}}{k}$$

$$\therefore ne^{kt} - \frac{\dot{n}_{H_2}}{k} e^{kt} = n_0 - \frac{\dot{n}_{H_2}}{k}$$

and solving for n :

$$n = \left(n_0 - \frac{\dot{n}_{H_2}}{k}\right) e^{-kt} + \frac{\dot{n}_{H_2}}{k}$$

$$\begin{aligned} \therefore \frac{dn}{dt} &= -k \left(n_0 - \frac{\dot{n}_{H_2}}{k}\right) e^{-kt} \\ &= (\dot{n}_{H_2} - kn_0) e^{-kt} \end{aligned}$$

Overall H_2 Balancein: $\dot{n}_{H_2}$ out: $\dot{n}_{H_2} y$ Accum: $\frac{d(ny)}{dt}$

$$n \frac{dy}{dt} + y \frac{dn}{dt} = \dot{n}_{H_2} - yn k$$

$$n \frac{dy}{dt} + y (\dot{n}_{H_2} - kn_0) e^{-kt} + yn k - \dot{n}_{H_2} = 0$$

not exact, $\therefore$ need Integration Factor, μ

$$\therefore \frac{\partial M}{\partial y} = (\dot{n}_{H_2} - kn_0)e^{-kt} + nk$$

$$\frac{\partial M}{\partial t} = (\dot{n}_{H_2} - kn_0)e^{-kt}$$

$$\frac{d\mu}{dt} = k\mu$$

$$\therefore \mu = e^{kt}$$

$\therefore$ Multiplying each term by μ ,

$$ne^{kt} \frac{dy}{dt} + y(\dot{n}_{H_2} - kn_0) + ynk e^{kt} - \dot{n}_{H_2} e^{kt} = 0$$

checking "exactness"

$$\frac{\partial M^s}{\partial y} = (\dot{n}_{H_2} - kn_0) + nke^{kt} -$$

$$\frac{\partial N^s}{\partial t} = e^{kt} \frac{dn}{dt} + n \frac{d(e^{kt})}{dt}$$

$$= (\dot{n}_{H_2} - kn_0) + nke^{kt} - \underline{\text{exact}}$$

Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = y(\dot{n}_{H_2} - kn_0) + ynk e^{kt} - \dot{n}_{H_2} e^{kt}$$

$$= y(\dot{n}_{H_2} - kn_0) + yk \left[(n_0 - \frac{\dot{n}_{H_2}}{k}) e^{-kt} + \frac{\dot{n}_{H_2}}{k} \right] e^{kt} - \dot{n}_{H_2} e^{kt}$$

$$= y(\cancel{\dot{n}_{H_2}} - kn_0) + yk(\cancel{n_0} - \frac{\dot{n}_{H_2}}{k}) + y\dot{n}_{H_2} e^{kt} - \dot{n}_{H_2} e^{kt}$$

$$\therefore \psi = \frac{y\dot{n}_{H_2}}{k} e^{kt} = \frac{\dot{n}_{H_2}}{k} e^{kt} + h(y) = C \quad \text{General Soln}$$

and

$$\frac{\partial \Psi}{\partial y} = \frac{\dot{n}_{H_2}}{k} e^{kt} + h'(y)$$

$$\text{Setting equal to } \frac{\partial \Psi}{\partial y} = n e^{kt} = \left[\left(n_0 - \frac{\dot{n}_{H_2}}{k} \right) e^{-kt} + \frac{\dot{n}_{H_2}}{k} \right] e^{kt}$$

$$= \left(n_0 - \frac{\dot{n}_{H_2}}{k} \right) + \frac{\dot{n}_{H_2}}{k} e^{kt}$$

$$\therefore h'(y) = \left(n_0 - \frac{\dot{n}_{H_2}}{k} \right)$$

$$\text{and } h(y) = \left(n_0 - \frac{\dot{n}_{H_2}}{k} \right) y$$

$$\therefore y \frac{\dot{n}_{H_2}}{k} e^{kt} - \frac{\dot{n}_{H_2}}{k} e^{kt} + \left(n_0 - \frac{\dot{n}_{H_2}}{k} \right) y = C$$

Solving for C, at $t=0$ $y=y_0$

$$y_0 \frac{\dot{n}_{H_2}}{k} - \frac{\dot{n}_{H_2}}{k} + \left(n_0 - \frac{\dot{n}_{H_2}}{k} \right) y_0 = C$$

$$\therefore C = n_0 y_0 - \frac{\dot{n}_{H_2}}{k}$$

and

$$\therefore y \frac{\dot{n}_{H_2}}{k} e^{kt} - \frac{\dot{n}_{H_2}}{k} e^{kt} + \left(n_0 - \frac{\dot{n}_{H_2}}{k} \right) y = n_0 y_0 - \frac{\dot{n}_{H_2}}{k}$$

Solving for y:

$$y \left(\frac{\dot{n}_{H_2}}{k} e^{kt} + \left(n_0 - \frac{\dot{n}_{H_2}}{k} \right) \right) = n_0 y_0 - \frac{\dot{n}_{H_2}}{k} + \frac{\dot{n}_{H_2}}{k} e^{kt}$$

$$y \left(\frac{\dot{n}_{H_2}}{k} [e^{kt} - 1] + n_0 \right) = \frac{\dot{n}_{H_2}}{k} (e^{kt} - 1) + n_0 y_0$$

$$\therefore y = \frac{\left[\frac{\dot{n}_{H_2}}{k} (e^{kt} - 1) + n_0 y_0 \right]}{\left[\frac{\dot{n}_{H_2}}{k} (e^{kt} - 1) + n_0 \right]} \quad \leftarrow H_2 \text{ fraction}$$

change in P ,

$$n = \left(n_0 - \frac{\dot{n}_{H_2}}{k}\right)e^{-kt} + \frac{\dot{n}_{H_2}}{k} = \frac{PV}{RT}$$

$$P = \frac{RT}{V} \left[\left(n_0 - \frac{\dot{n}_{H_2}}{k}\right)e^{-kt} + \frac{\dot{n}_{H_2}}{k} \right]$$

$$PP_{H_2} = y_{H_2} P$$

No Accum Initial Conditions @ Steady State $\dot{H}_e = 1.4 \text{ SCFM}$
for various $\dot{V}_{ex}$

Overall Balance

in: $\dot{n}_{H_2} + \dot{n}_{He}$

$\dot{n}_{He}$ & $\dot{n}_{H_2}$ fixed

out: $\dot{n}_{ex}$

$$\dot{n}_{ex} = \dot{n}_{H_2} + \dot{n}_{He} = \frac{P\dot{V}_{ex}}{RT}$$

P, T @ actual conditions

$$\therefore P = (\dot{n}_{H_2} + \dot{n}_{He}) \frac{RT}{\dot{V}_{ex}}$$

H_2 Balance

in: $\dot{n}_{H_2}$

out: $\dot{n}_{ex} y_{H_2}$

$$\therefore \dot{n}_{H_2} = \dot{n}_{ex} y_{H_2}$$

$$y_{H_2} = \frac{\dot{n}_{H_2}}{\dot{n}_{ex}} = \frac{\dot{n}_{H_2}}{\dot{n}_{H_2} + \dot{n}_{He}}$$

Therefore, initial conditions for continued vacuum and shut off helium purge:

$$y_{H_2}^0 = \frac{\dot{n}_{H_2}}{\dot{n}_{H_2} + \dot{n}_{He}}$$

$$P^0 = (\dot{n}_{H_2} + \dot{n}_{He}) \frac{RT}{\dot{V}_{ex}}$$

$\therefore$ partial pressure H_2 :
at this point

$$PP_{H_2} = y^0 P^0 = \frac{\dot{n}_{H_2} RT}{\dot{V}_{ex}}$$

After helium purge shut off:

at steady state:

$$y_{H_2} = \frac{\dot{n}_{H_2}}{\dot{n}_{ex}} = \frac{\dot{n}_{H_2}}{\dot{n}_{H_2}} = 1$$

$$\therefore p_{pH_2} = y_{H_2} P = P = \frac{\dot{n}_{H_2} RT}{\dot{V}_{ex}} = \frac{\dot{n}_H RT}{\dot{V}_{ex}} \text{ (from pg 5)}$$

Therefore, the partial pressure of hydrogen will remain constant after helium purge is shut off.

Appendix O

Prob 15

$$V_{MIS} = 0.56 \text{ ft}^3$$

$$y_{H_2}^0 = 0.01$$

Overall Balance

$$\text{in: } \dot{n}_{H_2}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{dn}{dt}$$

$$\frac{dn}{dt} = \dot{n}_{H_2}$$

$$n = \dot{n}_{H_2} t + n_0$$

Hydrogen Balance

$$\text{in: } \dot{n}_{H_2}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{d(ny)}{dt}$$

$$n \frac{dy}{dt} + y \frac{dn}{dt} = \dot{n}_{H_2}$$

$$n \frac{dy}{dt} + y \dot{n}_{H_2} - \dot{n}_{H_2} = 0$$

checking "exactness"

$$\frac{\partial M}{\partial y} = \dot{n}_{H_2}$$

$$\frac{\partial N}{\partial t} = \dot{n}_{H_2} \quad \checkmark \text{ exact}$$

Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = y \dot{n}_{H_2} - \dot{n}_{H_2}$$

$$\psi = \dot{n}_{H_2} (y-1)t + h(y) = C \quad \leftarrow \text{General Sol'n}$$

$$\frac{\partial \psi}{\partial y} = \dot{n}_{H_2} t + h'(y)$$

Setting equal to $\frac{\partial \Psi}{\partial y} = \dot{n}_{H_2} t + n_0$

$$\therefore h'(y) = n_0 \quad \text{and} \quad h(y) = n_0 y$$

$$\therefore \dot{n}_{H_2}(y-1)t + n_0 y = C$$

Solving for C, $C \text{ at } t=0 \quad y=y_0$

$$\therefore C = n_0 y_0$$

$$\therefore \dot{n}_{H_2} y t - \dot{n}_{H_2} t + n_0 y = n_0 y_0$$

and solving for y:

$$y(\dot{n}_{H_2} t + n_0) = \dot{n}_{H_2} t + n_0 y_0$$

$$\therefore y = \frac{(\dot{n}_{H_2} t + n_0 y_0)}{(\dot{n}_{H_2} t + n_0)}$$

$$n = \dot{n}_{H_2} t + n_0 = \frac{PV}{RT}$$

$$P = \frac{RT}{V} (\dot{n}_{H_2} t + n_0)$$

Appendix P

Prob. 16

1) Assume volume stagnant - no exit gas per purge

2) Assume volume at steady state
 $n_{H_2} = n_{ex}$

Find n_{H_2} :Receipt from K-Basins:

$P^0 = 5 \text{ psig}$ (initially leave K-Basins @ 5 psig) ^{assume}

$P_f = 150 \text{ psig}$ (design pressure)

$164.7 \text{ psia} - 19.7 \text{ psia} = 145 \text{ psia}$ (100% H_2 buildup in MCO/Cell associated gmoles H_2 : ^{MCO void vol.} ^{Crk void vol.}

$$n_{H_2} = \frac{PV}{RT} = \frac{(145 \text{ psia})(0.56 + 0.53) \text{ ft}^3}{(0.04259 \frac{\text{psia} \cdot \text{ft}^3}{\text{g mol} \cdot \text{K}})(283 \text{ K})} = 13.11 \text{ g mol } H_2$$

this amount is constrained by 10 SCFM vent into HVAC

checking if 10 SCFM is a constraint:

allowed

$$\dot{n}_{scfm} = \frac{(14.696 \text{ psia})(10 \text{ SCFM})}{(0.04259)(273)} = 12.64 \frac{\text{g mol } H_2}{\text{min}}$$

conservatively assuming 100% H_2

Therefore, limit to HVAC is $12.64 \frac{\text{g mol } H_2}{\text{min}}$

the available 13.11 g mol H_2 available upon receipt from K-Basins can only be purged into HVAC at a rate of 10 SCFM or 12.64 g mol/min

if this amount is assumed 100% H_2

then maximum H_2 rate into HVAC is $12.64 \frac{\text{g mol } H_2}{\text{min}}$

if limit extended to 40 SCFM,

$$\dot{n} = 12.64 \frac{\text{g mol } H_2}{\text{min}} \left(\frac{40 \text{ SCFM}}{10 \text{ SCFM}} \right) = 50.6 \frac{\text{g mol } H_2}{\text{min}}$$

P-2

Calculate number of moles vented to HVAC during mco/cask Purge/Vent Cycle @ (5.2 ~~35.2~~ psia (see Section 1.0))

Conservatively assume 100% H₂ (no He) in 20 psia gas in mco/cask void space. $\uparrow \Delta P$

$$\therefore \Delta n_{H_2} = \frac{\Delta PV}{RT} = \frac{(20 \text{ psia})[(0.53 + 0.56) \text{ ft}^3]}{(0.04259 \frac{\text{psia} \cdot \text{ft}^3}{\text{gmol} \cdot \text{K}})(293 \text{ K})} = 1.81 \text{ gmol H}_2$$

Since this is the amount of H₂ transferred to the HVAC in 1 vent cycle (very conservatively, since no He assumed)

Section 1 described the vent time (for the 20 psia mco/cask Purge/Vent Cycle) to approximately 44 seconds* or 0.732

$$\Delta t = \frac{V_1 \Delta P}{RT k \beta} = 0.732 \frac{\text{min}}{\text{cycle}} \quad V_1 = 0.53 \text{ ft}^3 \quad R = 0.04259 \frac{\text{psia} \cdot \text{ft}^3}{\text{gmol} \cdot \text{K}}$$

$$\Delta P = -20 \text{ psia}$$

$$T = 293 \text{ K}$$

$$k = \frac{V_1}{V_2} = \frac{0.53 \text{ ft}^3}{0.56 \text{ ft}^3} = 0.946$$

$$\beta = \frac{-(\dot{n}_{H_2} + \dot{n}_{He})}{(k+1)} = -1.27 \frac{\text{gmol}}{\text{min}}$$

$$\dot{n}_{He} = \left(\frac{PV}{RT} \right)_{\text{SCFM}} = \frac{(14.7)(1.9)}{RT} = 2.4 \frac{\text{gmol}}{\text{min}}$$

$$\therefore \frac{1.81 \text{ gmol H}_2}{\text{vent cycle}} \times \frac{\text{vent cycle}}{0.732 \text{ min}} = 2.47 \approx 2.5 \frac{\text{gmol H}_2}{\text{min}} \quad \checkmark \quad \text{ok}$$

$$2.5 < 12.64 \quad \text{ok} \quad \checkmark$$

R_{limit}

Overall Balance - over 1st minute purge

in: $\dot{n}_{H_2}$

out: $\dot{n}_{ex}$

Accum: 0 $\therefore \dot{n}_{ex} = \dot{n}_{H_2}$

H₂ Balance

in: $\dot{n}_{H_2}$

out: $\dot{n}_{ex} y$

Accum: $\frac{d(ny)}{dt}$

$$n \frac{dy}{dt} + y \frac{dn}{dt} \stackrel{ss.}{=} \dot{n}_{H_2} - \dot{n}_{ex} y$$

$$n \frac{dy}{dt} + \dot{n}_{ex} y - \dot{n}_{H_2} = 0$$

$$\text{since } \dot{n}_{ex} = \dot{n}_{H_2}$$

$$n \frac{dy}{dt} + \dot{n}_{H_2} y - \dot{n}_{H_2} = 0$$

$$\frac{\partial M}{\partial y} = \dot{n}_{H_2}$$

need integration factor, μ

$$\frac{d\mu}{dt} = \frac{\dot{n}_{H_2}}{n} \mu$$

$$\text{let } k = \frac{\dot{n}_{H_2}}{n}$$

$$\ln \mu = kt$$

$$\mu = e^{kt}$$

Multiplying all terms by e^{kt} ,

$$ne^{kt} \frac{dy}{dt} + e^{kt} n_{H_2} y - e^{kt} n_{H_2} = 0$$

Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = e^{kt} n_{H_2} y - e^{kt} n_{H_2}$$

$$\psi = \frac{n_{H_2} y}{k} e^{kt} - \frac{n_{H_2}}{k} e^{kt} + h(y) = C \quad \leftarrow \text{General Sol'n}$$

and

$$\frac{\partial \psi}{\partial y} = \frac{n_{H_2}}{k} e^{kt} + h'(y)$$

$$\text{Setting equal to } \frac{\partial \psi}{\partial y} = ne^{kt}$$

$$\therefore h'(y) = 0 \quad \text{and} \quad h(y) = 0$$

$$\therefore n y e^{kt} - n e^{kt} = C$$

Solving for C , at $t=0$ $y=y^0$

$$C = n y^0 - n = n(y^0 - 1)$$

$$\therefore n y e^{kt} - n e^{kt} = n(y^0 - 1)$$

and solving for y :

$$y = (y^0 - 1)e^{-kt} + 1$$

Appendix Q

Prob. 17

SCPM =

[1.4
2.1
3]

Pressure Rise

$$P^0 = 12 \text{ torr}$$

Overall Balance

$$\text{in: } \dot{n}_{He} + \dot{n}_{H_2}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{dn}{dt}$$

$$\frac{dn}{dt} = \dot{n}_{He} + \dot{n}_{H_2} - 0 = \Delta$$

$$\therefore n = \Delta t + n_0$$

H₂ Balance

$$\text{in: } \dot{n}_{H_2}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{d(ny)}{dt}$$

$$n \frac{dy}{dt} + y \frac{dn}{dt} = \dot{n}_{H_2}$$

$$n \frac{dy}{dt} + y\Delta - \dot{n}_{H_2} = 0$$

exactTherefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = y\Delta - \dot{n}_{H_2}$$

$$\psi = y\Delta t - \dot{n}_{H_2}t + h(y) = C$$

Q-2

General Soln

and $\frac{\partial \psi}{\partial y} = \alpha t + h'(y)$

Setting equal to $\frac{\partial \psi}{\partial y} = \alpha t + n_0$

$\therefore h'(y) = n_0$ and $h(y) = n_0 y$

$\therefore y \alpha t - n_{H_2} t + n_0 y = C$

Solving for C, $C \text{ at } t=0 \quad y=y_0$

$C = n_0 y_0$

$\therefore y \alpha t - n_{H_2} t + n_0 y = n_0 y_0$

Solving for y:

$y(\alpha t + n_0) = n_0 y_0 + n_{H_2} t$

$\therefore y = \frac{(n_{H_2} t + n_0 y_0)}{(\alpha t + n_0)}$

$n = \alpha t + n_0 = \frac{PV}{RT}$

$P = \frac{RT}{V} (\alpha t + n_0)$

Appendix R

Prob. 18

(1) Drawing _____ (2) Doc. No. _____ (3) Page 1 of 1
(4) Building _____ (5) Rev. _____ (6) Job No. _____
(7) Subject Air Inleak into CVD/MCO
(8) Originator John T. Irwin Date 6-4-97
(9) Checker A.L. Pasunwan Mike Pasunwan Date 6/5/97

- (10) The amount of air inleakage into the MCO to increase pressure 3 Torr in 1 hour from a base pressure of 0.5 Torr. @ 50°C = 323°K
Volume of MCO is 525 Liters (HNF-SN-SNF-TI-001, CVD Flowchart)

$$m = \frac{PV}{RT} = \frac{(3-0.5) \text{ Torr} \times 525 \text{ Liters}}{0.082 \frac{\text{atm-Liter}}{\text{g.mole-K}} \times 323^{\circ}\text{K} \times 760 \frac{\text{Torr}}{\text{atm}}}$$

$$m_{\text{air}} = 6.5203 \times 10^{-2} \text{ g.mole} \approx 1.89 \text{ g Air} @ 28.99 \frac{\text{g}}{\text{g.mol.}}$$

$$P_{\text{of Air @ STP}} = \frac{m}{V} = \frac{P}{RT} = \frac{1 \text{ atm.}}{0.082 \frac{\text{atm-Liter}}{\text{g.mole-K}} \times 270^{\circ}\text{K}}$$

$$= 4.5167 \times 10^{-2} \frac{\text{g.mole}}{\text{Liter}} = 1.309 \frac{\text{g}}{\text{Liter}}$$

$$\therefore \dot{V} = \frac{\dot{m}}{\rho} = \frac{1.89 \text{ g/hr}}{1.309 \text{ g/Liter}} = 1.444 \frac{\text{Liter}}{\text{hr}} \times \frac{1000 \text{ cc/Liter}}{3600 \text{ sec/hr}}$$

$$= 0.40 \text{ SCCS.}$$

$$\text{Design Leak Rate} \approx 1 \times 10^{-4} \text{ SCCS} \Rightarrow \text{S.F.} = 4000$$

Appendix S

H₂ Generation Rates per Fuel and Scrap BasketFuel surface area per fuel basket: 7,900 cm²UFuel surface area per scrap basket: 45,000 cm²UCase 1 - all fuel baskets (5)Total surface area: 5 (7,900 cm²U) = 39,500 cm²UBounding H₂ rateReference
HNF-2453, Rev. 0A Page 20

$$\text{Total H}_2 \text{ rate} = 39,500 \text{ cm}^2\text{U} \left(1.73 \times 10^2 \frac{\text{mg O}_2 \text{ wt gain}}{\text{cm}^2\text{U hr}} \right) / \left(2.05 \times 10^3 \frac{\text{g mol H}_2}{\text{mg O}_2 \text{ wt gain}} \right)$$

$$= 1.40 \frac{\text{g mol H}_2}{\text{hr}}$$

$$= 1.40 \frac{\text{g mol H}_2}{\text{hr}} \times \frac{1 \text{ hr}}{60 \text{ min}} = 0.023 \frac{\text{g mol H}_2}{\text{min}}$$

For each Fuel Basket

$$\frac{7,900 \text{ cm}^2\text{U}}{39,500 \text{ cm}^2\text{U}} = 0.20 \quad \therefore \dot{n}_{\text{H}_2} = 0.20 (0.023 \frac{\text{g mol H}_2}{\text{min}})$$

$$= 0.0046 \frac{\text{g mol}}{\text{min}} \quad \leftarrow$$

Case 2 - 4 fuel baskets, 1 scrap basketTotal surface area = 4(7,900 cm²U) + 45,000 cm²U = 76,600 cm²U

$$\therefore \text{Total H}_2 \text{ rate} = 0.023 \frac{\text{g mol H}_2}{\text{min}} \left(\frac{76,600 \text{ cm}^2\text{U}}{39,500 \text{ cm}^2\text{U}} \right) = 0.045 \frac{\text{g mol H}_2}{\text{min}}$$

$$\text{For Fuel Basket: } 0.045 \frac{\text{g mol H}_2}{\text{min}} \left(\frac{7,900 \text{ cm}^2\text{U}}{76,600 \text{ cm}^2\text{U}} \right) = 0.00464 \frac{\text{g mol H}_2}{\text{min}}$$

$$\text{For Scrap Basket: } 0.045 \frac{\text{g mol H}_2}{\text{min}} \left(\frac{45,000 \text{ cm}^2\text{U}}{76,600 \text{ cm}^2\text{U}} \right) = 0.0264 \frac{\text{g mol H}_2}{\text{min}}$$

Case 3 - 3 fuel baskets, 2 scrap baskets

$$\text{Total Surface area} = 3(7,900 \text{ cm}^2\text{u}) + 2(45,000 \text{ cm}^2\text{u}) = 113,700 \text{ cm}^2\text{u}$$

$$\text{Total } H_2 \text{ rate} = 0.023 \left(\frac{113,700}{39,500} \right) = 0.0662 \frac{\text{gmol } H_2}{\text{min}}$$

$$\text{For Fuel Basket: } 0.0662 \left(\frac{7,900}{113,700} \right) = 0.0046 \frac{\text{gmol } H_2}{\text{min}}$$

$$\text{For Scrap Basket: } 0.0662 \left(\frac{45,000}{113,700} \right) = 0.0262 \frac{\text{gmol } H_2}{\text{min}}$$

Case 4 - same as case 2

Case 5 - all fuel baskets (6)

$$\text{Total surface area} = 6(7,900 \text{ cm}^2\text{u}) = 47,400 \text{ cm}^2\text{u}$$

$$\text{Total } H_2 \text{ rate: } 0.023 \left(\frac{47,400}{39,500} \right) = 0.028 \frac{\text{gmol } H_2}{\text{min}}$$

$$\text{For Fuel Basket: } 0.028 \left(\frac{7,900}{47,400} \right) = 0.00467 \frac{\text{gmol } H_2}{\text{min}}$$

$$\text{For Scrap Basket: } 0.028 \left(\frac{45,000}{47,400} \right) = 0.0266 \frac{\text{gmol } H_2}{\text{min}}$$

Case 6 - 5 fuel baskets, 1 scrap basket

$$\text{Total surface area} = 5(7,900 \text{ cm}^2\text{u}) + 45,000 \text{ cm}^2\text{u} = 84,500 \text{ cm}^2\text{u}$$

$$\text{Total } H_2 \text{ rate} = 0.023 \left(\frac{84,500}{39,500} \right) = 0.0492 \frac{\text{gmol } H_2}{\text{min}}$$

$$\text{For Fuel Basket: } 0.0492 \left(\frac{7,900}{84,500} \right) = 0.0046 \frac{\text{gmol } H_2}{\text{min}}$$

$$\text{For Scrap Basket: } 0.0492 \left(\frac{45,000}{84,500} \right) = 0.0262 \frac{\text{gmol } H_2}{\text{min}}$$

Case 7 - 4 fuel baskets, 2 scrap baskets

$$\text{Total surface area} = 4(7,900) + 2(45,000) = 121,600 \text{ cm}^2$$

$$\text{Total } H_2 \text{ rate} = 0.023 \left(\frac{121,600}{39,500} \right) = 0.0708 \frac{\text{gmol}}{\text{min}}$$

$$\text{For Fuel Basket: } 0.0708 \left(\frac{7900}{121,600} \right) = 0.0046 \frac{\text{gmol}}{\text{min}}$$

$$\text{For Scrap Basket: } 0.0708 \left(\frac{45,000}{121,600} \right) = 0.0262 \frac{\text{gmol}}{\text{min}}$$

Case 8 - same as case 5

Initial H_2 fraction:

185 torr is the SCIC trip point

$$\therefore \frac{185 \text{ torr}}{760 \text{ torr}} \times 3.7\% = 2.12\% H_2$$

$$\approx 2\% H_2 \quad \leftarrow \text{initial } H_2 \%$$

22-141 50 SHEETS
22-142 100 SHEETS
22-144 200 SHEETS

ANALYTICAL CALCULATIONS

Page ____ of ____

Subject _____
 Originator _____ Date _____
 Checker _____ Date _____

Previous H_2 generation rates for MIA Fuel
 too conservative; therefore, altering for
 Case 5 through Case 8 as shown below:

For MK 1A

^{MK 1A}
 Max¹ SCRAP BASKET LOADING IS 575 kg AS COMPARED
 TO 980 kg FOR MK IV SCRAP BASKET

MAX MK 1A FUEL BASKET LOADING IS 48 ASSEMBLIES
 AS COMPARED TO ~~54~~ 54 ASSEMBLIES FOR MK IV
 FUEL BASKET.

Therefore,

$$\text{MK 1A SCRAP BASKET } H_2 \text{ RATE} = 0.0262 \left(\frac{575}{980} \right) = 0.0154 \frac{\text{gmol } H_2}{\text{min}}$$

$$\text{MK 1A FUEL BASKET } H_2 \text{ RATE} = 0.00469 \left(\frac{48}{54} \right) = 0.00412 \frac{\text{gmol } H_2}{\text{min}}$$

Case 1 - 5 Fuel Baskets - No Scrap Baskets

Total MCO void volume = 499 L

$$5,104 \text{ L Annulus void volume} \times 5 = 25,520 \text{ L}$$

$$36,402 \text{ L Gap vol. between baskets} \times 4 = 145,608 \text{ L}$$

$$60,899 \text{ L void volume above baskets} \times 1 = 60,899 \text{ L (Top void space)}$$

$$53,395 \text{ L void volume of FB} \times 5 = 266,975 \text{ L}$$

499 L

Case 2 - 4 Fuel Baskets - 1 Scrap Basket

Total MCO void volume = 519 L

$$5,037 \text{ L Annulus void volume} \times 5 = 25,185 \text{ L}$$

$$35,924 \text{ L Gap vol. between baskets} \times 4 = 143,696 \text{ L}$$

$$24,174 \text{ L Top void space} \times 1 = 24,174 \text{ L}$$

$$115,177 \text{ L void vol. Scrap Basket} \times 1 = 115,177 \text{ L}$$

$$52,693 \text{ L void vol. of FB} \times 4 = 210,772 \text{ L}$$

519 L

Case 3 - 3 Fuel Baskets - 2 Scrap Baskets

Total MCO void volume = 538 L

$$4,967 \text{ L Annulus void vol.} \times 5 = 24,835 \text{ L}$$

$$35,426 \text{ L Gap vol. between baskets} \times 3 = 106,279 \text{ L (insignificant gap vol. between bottom scrap and fuel basket)}$$

$$23,839 \text{ L Top void space} \times 1 = 23,839 \text{ L}$$

$$113,580 \text{ L void vol. SB} \times 2 = 227,160 \text{ L}$$

$$51,963 \text{ L void vol. FB} \times 3 = 155,889 \text{ L}$$

538 L

Case 4 - 4 Fuel Baskets - 1 Scrap Basket - Nominal Loading

Total MCO void volume = 527 L

$$\begin{aligned}
 5,114 \text{ L Annulus void volume} \times 5 &= 25,57 \text{ L} \\
 36,477 \text{ L Gap vol. between baskets} \times 4 &= 145,908 \text{ L} \\
 24,547 \text{ L Top Void Space} \times 1 &= 24,547 \text{ L} \\
 116,952 \text{ L void vol. Scrap Basket} \times 1 &= 116,952 \text{ L} \\
 53,505 \text{ L void vol. of FB} \times 4 &= 214,020 \text{ L} \\
 \hline
 &527 \text{ L}
 \end{aligned}$$

Case 5 - 6 Fuel Baskets - No Scrap Baskets

Total MCO void volume = 524 L

$$\begin{aligned}
 5,905 \text{ L Annulus void volume} \times 6 &= 35,43 \text{ L} \\
 29,954 \text{ L Gap vol. between baskets} \times 5 &= 149,77 \text{ L} \\
 66,089 \text{ L Top Void Space} \times 1 &= 66,089 \text{ L} \\
 45,452 \text{ L void vol. of FB} \times 6 &= 272,712 \text{ L} \\
 \hline
 &524 \text{ L}
 \end{aligned}$$

Case 6 - 5 Fuel Baskets - 1 Scrap Basket

Total MCO void volume = 543 L

$$\begin{aligned}
 5,690 \text{ L Annulus void volume} \times 6 &= 34,14 \text{ L} \\
 28,865 \text{ L Gap vol. between baskets} \times 5 &= 144,325 \text{ L} \\
 45,681 \text{ L Top Void Space} \times 1 &= 45,681 \text{ L} \\
 99,853 \text{ L void vol. of SB} \times 1 &= 99,853 \text{ L} \\
 43,800 \text{ L void vol. of FB} \times 5 &= 219 \text{ L} \\
 \hline
 &543 \text{ L}
 \end{aligned}$$

Case 7 - 4 Fuel Baskets - 2 Scrap Baskets

Total MCO void volume = 563 L

$$5,513 \text{ L Annulus void vol.} \times 6 = 33,078 \text{ L}$$

$$27,969 \text{ L Gap vol. between baskets} \times 4 = 111,976 \text{ L}$$

$$54,785 \text{ L Top Void Space} \times 1 = 54,785 \text{ L}$$

$$96,751 \text{ L void vol. Scrap Basket} \times 2 = 193,502 \text{ L}$$

$$42,439 \text{ L void vol. FB} \times 4 = 169,756 \text{ L}$$

563 L

Case 8 - 5 Fuel Baskets - 1 Scrap Basket - Nominal Loading

Total MCO void volume = 549 L

$$5,742 \text{ L Annulus void vol.} \times 6 = 34,452 \text{ L}$$

$$29,131 \text{ L Gap vol. between baskets} \times 5 = 145,655 \text{ L}$$

$$46,102 \text{ L Top Void Space} \times 1 = 46,102 \text{ L}$$

$$100,772 \text{ L void vol. Scrap Basket} \times 1 = 100,772 \text{ L}$$

$$44,203 \text{ L void vol. FB} \times 5 = 221,015 \text{ L}$$

549 L

Case 1

Maximum Fuel Loading MK II

5 FB

FB void space:

53.778 L

Sector fraction

0.5664

Annulus:

5.062 L

0.0533

Gap:

36.101 L

0.3802

Total Void Vol. per Sector:

94.941 L

4 sectors

Top Fuel Basket void space:

53.778 L

Sector fraction

0.4510

Annulus:

5.062 L

0.0424

Gap:

60.395 L

0.5065

119.235 L

1 sector

Total Void Vol.:

$$94.941 \frac{\text{L}}{\text{Sector}} \times 4 \text{ sectors} = 379.764 \text{ L}$$

+

$$119.235 \frac{\text{L}}{\text{Sector}} \times 1 \text{ sector} = \frac{119.235 \text{ L}}{499 \text{ L}}$$

Case 2

Maximum Particulate Loading MIC IV 4 FB 1 SB

FB void space:	53.177 L	<u>Fraction of Sector</u> 0.5664
----------------	----------	-------------------------------------

Annulus:	5.005 L	0.0533
----------	---------	--------

Gap:	35.648 L	<u>0.3802</u>
------	----------	---------------

Total Void Vol. per Sector:	93.88 L	4 sectors
-----------------------------	---------	-----------

SB void space:	114.452 L	<u>Fraction of Sector</u> 0.7977
----------------	-----------	-------------------------------------

Annulus:	5.005 L	0.03488
----------	---------	---------

Gap:	24.022 L	<u>0.1674</u>
------	----------	---------------

Total Void Vol. per Sector:	143.479 L	1 sector
-----------------------------	-----------	----------

Total Void Volume: $93.88 \text{ L} \times \frac{4 \text{ sectors}}{\text{Sector}} = 375.52 \text{ L}$

+ $143.479 \text{ L} \times \frac{1 \text{ sector}}{\text{Sector}} = 143.479 \text{ L}$

Total: 519 L

22-141 50 SHEETS
22-142 100 SHEETS
22-144 200 SHEETS

Case 3

Maximum Particulate Loading MKIV 3 FB 2 SB

		<u>Fraction of sector</u>	
FB void space:	52,535 L	0.5664	
Annulus:	4,945 L	0.0533	
Gap:	<u>35,267 L</u>	<u>0.3802</u>	
Total Void Vol. per Sector:	92.747 L		3 Sectors
<u>Top</u> SB void space:	113,070 L	0.7977	
Annulus:	4,945 L	0.03489	
Gap:	<u>23,732 L</u>	<u>0.1674</u>	
	141.747 L		1 Sector
<u>Bottom</u> SB void space:	113,070 L	0.9581	
Annulus:	4,945 L	0.0419	
Gap:	<u>0</u>		
	118.015 L		1 Sector
Total Void Vol:	$92.747 \frac{\text{L}}{\text{sector}} \times 3 \text{ sectors} = 278.241 \text{ L}$		
	$+ 141.747 \frac{\text{L}}{\text{sector}} \times 1 \text{ sector} = 141.747 \text{ L}$		
	$+ 118.015 \frac{\text{L}}{\text{sector}} \times 1 \text{ sector} = 118.015 \text{ L}$		
		<u>538 L</u>

Fraction Void Space per Sector

Case 4

FB void space: 53.997 L 0.5664

Annulus: 5.082 L 0.0533

Gap: 36.248 L 0.3802

Total Void Vol. per Sector: 95.327 L

4 sectors

SB void space: 116.217 L 0.7977

Annulus: 5.082 L 0.0349

Gap: 24.343 L 0.1674

Total Void Vol. per Sector: 145.642 L

1 sector

Total Void Volume: 527 L

Maximum Loading MKII 5 FB 0 SB

Fraction Void Space per Sector

FB void space: 53.779 L 0.5664

Annulus: 5.062 L 0.0533

Gap: 36.101 L 0.3802

94.941 L

4 sectors

top

FB void space: 53.779 L

Annulus: 5.062 L

Gap: 24.294 L

83.134 L

1 sector

Case 5 Maximum Fuel Loading MK 1A 6 FB

FB void space: 45.999 L Sector Fraction
0.5652

Annulus: 5.827 L 0.0716

Gap: 29.563 L 0.3632

Total Void Vol. per Sector: 81.389 L

5 sectors

Top FB void space: 45.999 L 0.3930

Annulus: 5.827 L 0.04979

Gap: 65.225 L 0.5572

Total Void Vol. per Sector: 117.051 L

1 sector

Total Void Volume: $81.389 \frac{\text{L}}{\text{Sector}} \times 5 \text{ sectors} = 406.945 \text{ L}$

+ $117.051 \frac{\text{L}}{\text{Sector}} \times 1 \text{ sector} = 117.051 \text{ L}$
524 L

22-141 50 SHEETS
22-142 100 SHEETS
22-144 200 SHEETS

Case 6

Maximum Particulate Loading - MK 1A 5FB 1SB

FB void space: 44,458 L

Fraction Void Space per Sec

0.5652

Annulus: 5.632 L

0.0716

Gap: 28.572 L

0.3632

Total Void Volume per Sector: 78.662 L

5 Sector

SB void space: 98.838 L

0.6603

Annulus: 5.632 L

0.0376

Gap: 45.217 L

0.3021

149.687 L

1 Sector

Total void volume: $78.662 \frac{\text{L}}{\text{Sector}} \times 5 \text{ sectors} = 393.31 \text{ L}$

+

$149.687 \frac{\text{L}}{\text{Sector}} \times 1 \text{ sector} = 149.687 \text{ L}$

543 L

Case 7

Maximum Particulate Loading- MKIA 4FB 2SB

			<u>Fraction Void Space Per Sec.</u>	
FB void space:	43,188 L		0.5652	
Annulus:	5,471 L		0.0716	
Gap:	27,756 L		0.3632	
Total Void Vol. per Sector:	76,415 L			4 sectors
Bottom SB void space:	96,014 L		0.9461	
Annulus:	5,471 L		0.0539	
Gap:	insignificant		~0	
Total	101,485 L			1 sector
Top SB void space:	96,014 L		0.6160	
Annulus:	5,471 L		0.0351	
Gap:	54,368 L		0.3449	
	155,853 L			1 sector
Total void volume:				
	$76,415 \frac{\text{L}}{\text{sector}}$	$\times$	4 sectors	$= 305.66 \text{ L}$
+	$101,485 \frac{\text{L}}{\text{sector}}$	$\times$	1 sector	$= 101.435 \text{ L}$
+	$155,853 \frac{\text{L}}{\text{sector}}$	$\times$	1 sector	$= 155.853 \text{ L}$
				<u>563 L</u>

Case B

Nominal Loadings - MKIA

5FB

1SB

FB void space:	44,968 L	<u>Fraction Void Space Per Sector</u> 0.5652
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Annulus:	5,684 L	0.0716
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Gap:	<u>28,835 L</u>	<u>0.3632</u>
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79,387 L

5 sectors

SB void space:	99,748 L	0.6603
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Annulus:	5,684 L	0.0376
----------	---------	--------

Gap:	<u>45,633 L</u>	<u>0.3021</u>
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151,065 L

1 sector

Total Void Volume:

$$79.387 \frac{\text{L}}{\text{sector}} \times 5 \text{ sectors} = 396.935 \text{ L}$$

+

$$151.065 \frac{\text{L}}{\text{sector}} \times 1 \text{ sector} = 151.065 \text{ L}$$

 548 L

Overall Balance around Fuel Basket #1

$$\text{in: } \dot{n}_{H_2} + \dot{n}_{E1}$$

$$\dot{n}_{E1} = 0.20 \dot{n}_{H_2}$$

$$\text{out: } \dot{n}_{F1}$$

$$\text{Accum: } \frac{dn_{A1}}{dt}$$

$$\frac{dn_{A1}}{dt} = \dot{n}_{H_2} + \dot{n}_{E1} - \dot{n}_{F1} = \Delta_{A1}$$

$$n_{A1} = \Delta_{A1} t + n_{A1}^0 = \frac{PV_A}{RT}$$

$$\Delta P = \frac{\Delta_{A1} RT}{V_A}$$

Setting equal to overall MCO balance, i.e. $\Delta P_{F02} = \Delta P_{MCO}$

$$\frac{\Delta_{A1} RT}{V_A} = \Delta \frac{RT}{V_{MCO}}$$

$$\Delta_{A1} = \left(\frac{V_A}{V_{MCO}} \right) \Delta$$

$$\dot{n}_{H_2} + \dot{n}_{E1} - \dot{n}_{F1} = \left(\frac{V_A}{V_{MCO}} \right) \Delta$$

$$\dot{n}_{F1} = \dot{n}_{H_2} + \dot{n}_{E1} - \left(\frac{V_A}{V_{MCO}} \right) \Delta$$

Overall Balance around Annulus 1in: $\dot{n}_{O1}$ out: $\dot{n}_{G1}$ Accum: $\frac{dn_{B1}}{dt}$

$$\frac{dn_{B1}}{dt} = \dot{n}_{O1} - \dot{n}_{G1} = \Delta_{B1}$$

$$\therefore n_{B1} = \Delta_{B1} t + n_{B1}^0 = \frac{PV_{B1}}{RT}$$

$$\therefore \Delta P = \frac{\Delta_{B1} RT}{RT}$$

Setting equal to overall mco balance,

$$\frac{\Delta_{B1} RT}{V_B} = \frac{\Delta_{TCD} \Delta}{V_{mco}}$$

$$\therefore \Delta_{B1} = \left(\frac{V_{B1}}{V_{mco}} \right) \Delta$$

$$\therefore \dot{n}_{G1} = \dot{n}_{O1} - \left(\frac{V_{B1}}{V_{mco}} \right) \Delta$$

Overall Balance around Gap #1

$$\text{in: } \dot{m}_{F1} + \dot{m}_{G1}$$

$$\text{out: } \dot{m}_{EX1}$$

$$\text{Accum: } \frac{d m_G}{dt}$$

$$\frac{d m_G}{dt} = \dot{m}_{F1} + \dot{m}_{G1} - \dot{m}_{EX1} = \dot{\alpha}_{G1}$$

$$m_G = \dot{\alpha}_{G1} t + m_{G1}^o$$

22-141 50 SHEETS
22-142 100 SHEETS
22-144 200 SHEETS

O₂ balance around FB #1

in: 0

out: $\dot{n}_{A1} y_{A1}$ Accum: $\frac{d(n_{A1} y_{A1})}{dt}$

$$\dot{n}_{A1} \frac{dy_{A1}}{dt} + y_{A1} \frac{d\dot{n}_{A1}}{dt} = 0 - \dot{n}_{F1} y_{A1}$$

$$\dot{n}_{A1} \frac{dy_{A1}}{dt} + \dot{n}_{A1} y_{A1} + \dot{n}_{F1} y_{A1} = 0$$

checking "exactness"

$$\frac{\partial M}{\partial y} = \dot{n}_{A1} + \dot{n}_{F1}$$

$$\frac{\partial N}{\partial t} = \dot{n}_{A1}$$

not exact

Need Integration Factor,

$$\frac{d\mu}{dt} = \frac{\dot{n}_{F1}}{\dot{n}_{A1}} \mu$$

$$\int \frac{d\mu}{\mu} = \dot{n}_{F1} \int \frac{1}{(\dot{n}_{A1} t + n_1^0)} dt$$

$$\ln \mu = \frac{\dot{n}_{F1}}{\dot{n}_{A1}} \ln \dot{n}_{A1}$$

$$\text{let } \delta_{A1} = \frac{\dot{n}_{F1}}{\dot{n}_{A1}}$$

$$\mu = \dot{n}_{A1}^{\delta_{A1}}$$

Multiplying all terms by $\dot{n}_{A1}^{\delta_{A1}}$

$$\dot{n}_{A1}^{\delta_{A1}+1} \frac{dy_{A1}}{dt} + \dot{n}_{A1}^{\delta_{A1}} (\dot{n}_{A1} y_{A1} + \dot{n}_{F1} y_{A1}) = 0$$

Therefore, there exists ψ such that:

$$\frac{\partial \psi}{\partial t} = \dot{n}_{A1}^{\delta_{A1}} (\dot{n}_{A1} y_{A1} + \dot{n}_{F1} y_{A1})$$

$$\psi = \frac{(\dot{n}_{A1}^{\delta_{A1}+1} y_{A1} + \dot{n}_{F1} \dot{n}_{A1}^{\delta_{A1}} y_{A1})}{\dot{n}_{A1}(\delta_{A1}+1)} + h(y_{A1}) = C \quad \text{General Sol'n}$$

and taking

$$\frac{\partial \psi}{\partial y_{A1}} = \frac{(d_{A1} + n_{E1}) n_{A1}^{\delta_{A1}+1}}{d_{A1}(\delta_{A1}+1)} + h'(y_{A1})$$

note: $\frac{(d_{A1} + n_{E1})}{d_{A1}(\delta_{A1}+1)} = 1$

$$\delta_{A1} = \frac{n_{E1}}{d_{A1}}$$

$\therefore$ setting $\frac{\partial \psi}{\partial y_{A1}} = n_{A1}^{\delta_{A1}+1}$

$\therefore h'(y_{A1}) = 0$ and $h(y_{A1}) = 0$

Substituting into general sol'n and solving for C, $C t=0$
 $y_{A1} = y_{A1}^0$

$C = n_{A1}^{\delta_{A1}+1} y_{A1}^0$
 and therefore,

$$y_{A1} n_{A1}^{\delta_{A1}+1} = n_{A1}^0 y_{A1}^0$$

and

$$y_{A1} = \frac{n_{A1}^{\delta_{A1}+1}}{n_{A1}^0} y_{A1}^0$$

$$y_{A1} = \left(\frac{n_{A1}^0}{(d_{A1} + n_{A1}^0)} \right) y_{A1}^0$$

$$y_{A1} = \left[\frac{n_{A1}^0}{(d_{A1} + n_{A1}^0)} \right]^{\delta_{A1}+1} y_{A1}^0$$

← D_2 sol'n during P increase
 in FB #1

O₂ Balance in Annulus #1

• identical to FB1 balance

$$y_{B2} = \left[\frac{n_{B1}^0}{(\alpha_{B1} t + n_{B1}^0)} \right]^{\delta_{B1} + 1} y_{B1}^0$$

where: $y_{B2}^0 = 1.0$

$$\alpha_{B2} = \frac{dn_{B1}}{dt} = \dot{n}_{O1} - \dot{n}_{G1}$$

$$\delta_{B1} = \frac{\dot{n}_{O2}}{\alpha_{B1}}$$

$$\dot{n}_{G2} = \dot{n}_{O1} - \left(\frac{V_B}{V_{m10}} \right) \alpha$$

$$\dot{n}_{O1} = 0.80 \dot{n}_{H2}$$

$$V_B = 0.05 \left(\frac{13 \text{ ft}^3}{5} \right) \quad V_{m10} = 13 \text{ ft}^3$$

↑ assume 5% volume from void spaces of Fuel Basket, Gap, and Annulus.

$$\alpha = 4 \dot{n}_{H2} + \dot{n}_{He}$$

O₂ Balance around Gap #1

in: $\dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1}$

out: $\dot{n}_{ex1} y_{C1}$

Accum: $\frac{d(n_{C2} y_{C1})}{dt}$

$$n_{C1} \frac{dy_{C1}}{dt} + y_{C1} \frac{dn_{C1}}{dt} = \dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1} - \dot{n}_{ex1} y_{C1}$$

$$n_{C1} \frac{dy_{C1}}{dt} + y_{C1} \alpha_{C1} + \dot{n}_{ex1} y_{C1} - \dot{n}_{F1} y_{A1} - \dot{n}_{G1} y_{B1} = 0$$

↑
N

"checking exactness"

$$n_{C1} = \alpha_{C1} t + n_{C1}^0$$

$$\frac{\partial M}{\partial y_{C1}} = \alpha_{C1} + \dot{n}_{ex1}$$

$$\frac{\partial N}{\partial t} = \alpha_{C1}$$

Need Integration Factor

$$\frac{d\mu}{dt} = \frac{\dot{n}_{ex1}}{n_{c1}} \mu$$

$$\alpha_{c1} = \dot{n}_{F1} + \dot{n}_{G1} - \dot{n}_{ex1}$$

$$\int \frac{d\mu}{\mu} = \dot{n}_{ex1} \int \frac{1}{(\alpha_{c1}t + n_{c1}^0)} dt$$

$$\ln \mu = \frac{\dot{n}_{ex1}}{\alpha_{c1}} \ln n_{c1}$$

$$\text{let } \gamma_{c1} = \frac{\dot{n}_{ex1}}{\alpha_{c1}}$$

$$\mu = n_{c1}^{\gamma_{c1}}$$

Therefore, multiply all terms by $n_{c1}^{\gamma_{c1}}$,

$$n_{c1}^{\gamma_{c1}+1} \frac{dy_{c1}}{dt} + n_{c1}^{\gamma_{c1}} \left[y_{c1}(\alpha_{c1} + \dot{n}_{ex1}) - \underbrace{y_{A1} \dot{n}_{F1}}_{f(t)} - \underbrace{y_{B1} \dot{n}_{G1}}_{f(t)} \right] = 0$$

and there exists Ψ such that:

$$\frac{\partial \Psi}{\partial y_{c1}} = n_{c1}^{\gamma_{c1}} \left[y_{c1}(\alpha_{c1} + \dot{n}_{ex1}) - \dot{n}_{F1} \left[y_{A1}^0 \left(\frac{n_{A1}^0}{\alpha_{A1}t + n_{A1}^0} \right) \right]^{\gamma_{A1}+1} - \dot{n}_{G1} \left[y_{B1}^0 \left(\frac{n_{B1}^0}{\alpha_{B1}t + n_{B1}^0} \right) \right]^{\gamma_{B1}+1} \right]$$

too difficult to solve
need numerical sol'n

$$\therefore \frac{dy_{c1}}{dt} = \frac{1}{n_{c1}} \left[\dot{n}_{ex1} y_{c1} - \alpha_{c1} y_{c1} + \dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1} \right]$$

Overall Balance around Fuel Basket #2

identical to #1 but with #2 subscript,

$$\frac{dn_{f2}}{dt} = \dot{n}_{H2} + \dot{n}_{E2} - \dot{n}_{F2} = \Delta_{f2}$$

$$\text{note: } \dot{n}_{E2} = 0.20 \dot{n}_{E1}$$

$$\therefore n_{f2} = \Delta_{f2} t + n_{f2}^0 = \frac{P V_{f2}}{RT}$$

$$\therefore \Delta P = \frac{\Delta_{f2} RT_t}{V_{f2}}$$

Setting equal to overall MCO ΔP ,

$$\Delta P = \frac{\Delta RT_t}{V_{mco}}$$

$$\frac{\Delta_{f2} RT_t}{V_{f2}} = \frac{\Delta RT_t}{V_{mco}}$$

$$\Delta_{f2} = \left(\frac{V_{f2}}{V_{mco}} \right) \Delta$$

$$\dot{n}_{H2} + \dot{n}_{E2} - \dot{n}_{F2} = \left(\frac{V_{f2}}{V_{mco}} \right) \Delta$$

$$\therefore \dot{n}_{F2} = \dot{n}_{H2} + \dot{n}_{E2} - \left(\frac{V_{f2}}{V_{mco}} \right) \Delta$$

Overall Balance around Annulus 2

as before, using subscript #2,

$$\frac{dn_{B2}}{dt} = \dot{n}_{O2} - \dot{n}_{E2} = \Delta_{B2}$$

$$\therefore n_{B2} = \Delta_{B2} t + n_{B2}^0 = \frac{P V_{B2}}{RT}$$

$$\therefore \Delta P = \frac{\Delta_{B2} RT_t}{V_{B2}}$$

Setting equal to overall Annulus #2

$$\Delta_{B2} = \left(\frac{V_{B2}}{V_{mco}} \right) \Delta$$

$$\therefore \dot{n}_{E2} = \dot{n}_{O2} - \left(\frac{V_{B2}}{V_{mco}} \right) \Delta \quad \text{S-24}$$

Overall Balance around Gap #2

as before, using subscript #2,

$$\frac{dn_{C2}}{dt} = \dot{n}_{F2} + \dot{n}_{G2} - \dot{n}_{E2} = \Delta_{C2}$$

$$\therefore n_{C2} = \Delta_{C2} t + n_{C2}^0$$

O₂ Balance around FB #2

in: $\dot{n}_{E2} y_{C1}$

out: $\dot{n}_{F2} y_{A2}$

Accum. $\frac{d(n_{A2} y_{A2})}{dt}$

$$n_{A2} \frac{dy_{A2}}{dt} + y_{A2} \frac{dn_{A2}}{dt} = \dot{n}_{E2} y_{C1} - \dot{n}_{F2} y_{A2}$$

$$\therefore \frac{dy_{A2}}{dt} = \frac{1}{n_{A2}} [\dot{n}_{E2} y_{C1} - \Delta_{A2} y_{A2} - \dot{n}_{F2} y_{A2}];$$

O₂ Balance around Annulus #2

in: $\dot{n}_{D2} y_{C1}$

out: $\dot{n}_{G2} y_{B2}$

Accum. $\frac{d(n_{B2} y_{B2})}{dt}$

$$n_{B2} \frac{dy_{B2}}{dt} + y_{B2} \frac{dn_{B2}}{dt} = \dot{n}_{D2} y_{C1} - \dot{n}_{G2} y_{B2}$$

$$\therefore \frac{dy_{B2}}{dt} = \frac{1}{n_{B2}} [\dot{n}_{D2} y_{C1} - \Delta_{B2} y_{B2} - \dot{n}_{G2} y_{B2}];$$

O₂ Balance around Gap #2

$$\text{in: } \dot{n}_{F2} y_{A2} + \dot{n}_{G2} y_{B2}$$

$$\text{out: } \dot{n}_{E2} y_{C2}$$

$$\text{Accum: } \frac{d(n_{C2} y_{C2})}{dt}$$

$$n_{C2} \frac{dy_{C2}}{dt} + y_{C2} \frac{dn_{C2}}{dt} = \dot{n}_{F2} y_{A2} + \dot{n}_{G2} y_{B2} - \dot{n}_{E2} y_{C2}$$

$$\therefore \frac{dy_{C2}}{dt} = \frac{1}{n_{C2}} [\dot{n}_{F2} y_{A2} + \dot{n}_{G2} y_{B2} - \dot{n}_{E2} y_{C2} - d_{C2} y_{C2}] ;$$

O₂ Balance around FBA #3

in: $\dot{n}_{E3} y_{O2}$

$\dot{n}_{E3} = 0.20 \dot{n}_{E12}$

out: $\dot{n}_{F3} y_{A3}$

Accum: $\frac{d(n_{A3} y_{A3})}{dt}$

$$n_{A3} \frac{dy_{A3}}{dt} + y_{A3} \frac{dn_{A3}}{dt} = \dot{n}_{E3} y_{O2} - \dot{n}_{F3} y_{A3}$$

$$\therefore \frac{dy_{A3}}{dt} = \frac{1}{n_{A3}} [\dot{n}_{E3} y_{O2} - \dot{n}_{F3} y_{A3} - \alpha_{A3} y_{A3}]$$

as before,

$$\dot{n}_{F3} = \dot{n}_{H2} + \dot{n}_{E3} - \left(\frac{V_{A3}}{V_{mro}} \right) \alpha$$

$$\alpha_{A3} = \dot{n}_{H2} + \dot{n}_{E3} - \dot{n}_{F3}$$

O₂ Balance around Annulus #3

in: $\dot{n}_{D3} y_{O2}$

$\dot{n}_{D3} = 0.80 \dot{n}_{E12}$

out: $\dot{n}_{G3} y_{B3}$

Accum: $\frac{d(n_{B3} y_{B3})}{dt}$

$$n_{B3} \frac{dy_{B3}}{dt} + y_{B3} \frac{dn_{B3}}{dt} = \dot{n}_{D3} y_{O2} - \dot{n}_{G3} y_{B3}$$

$$\therefore \frac{dy_{B3}}{dt} = \frac{1}{n_{B3}} [\dot{n}_{D3} y_{O2} - \dot{n}_{G3} y_{B3} - \alpha_{B3} y_{B3}]$$

$$\alpha_{B3} = \dot{n}_{D3} - \dot{n}_{G3}$$

$$\dot{n}_{G3} = \dot{n}_{D3} - \left(\frac{V_{B3}}{V_{mro}} \right) \alpha$$

O₂ Balance around Gap #3

$$\text{in: } \dot{n}_{F3} y_{A3} + \dot{n}_{G3} y_{B3}$$

$$\text{out: } \dot{n}_{E3} y_{C3}$$

$$\text{Accum: } \frac{d(\dot{n}_{C3} y_{C3})}{dt}$$

$$\dot{n}_{C3} \frac{dy_{C3}}{dt} + y_{C3} \frac{d\dot{n}_{C3}}{dt} = \dot{n}_{F3} y_{A3} + \dot{n}_{G3} y_{B3} - \dot{n}_{E3} y_{C3}$$

$$\frac{dy_{C3}}{dt} = \frac{1}{\dot{n}_{C3}} [\dot{n}_{F3} y_{A3} + \dot{n}_{G3} y_{B3} - \dot{n}_{E3} y_{C3} - \dot{n}_{C3} y_{C3}]$$

$$\text{as before, } \dot{n}_{C3} = \dot{n}_{F3} + \dot{n}_{G3} - \dot{n}_{E3}$$

O₂ Balance around FB #4

$$\text{in: } \dot{n}_{E4} y_{C3}$$

$$\dot{n}_{E4} = 0.20 \dot{n}_{E3}$$

$$\text{out: } \dot{n}_{F4} y_{A4}$$

$$\text{Accum: } \frac{d(\dot{n}_{A4} y_{A4})}{dt}$$

$$\dot{n}_{A4} \frac{dy_{A4}}{dt} + y_{A4} \frac{d\dot{n}_{A4}}{dt} = \dot{n}_{E4} y_{C3} - \dot{n}_{F4} y_{A4}$$

$$\frac{dy_{A4}}{dt} = \frac{1}{\dot{n}_{A4}} [\dot{n}_{E4} y_{C3} - \dot{n}_{F4} y_{A4} - \dot{n}_{A4} y_{A4}]$$

as before,

$$\dot{n}_{A4} = \dot{n}_{H2} + \dot{n}_{E4} - \dot{n}_{F4}$$

$$\dot{n}_{F4} = \dot{n}_{H2} + \dot{n}_{E4} - \left(\frac{V_{A9}}{V_{m10}} \right) \dot{n}_{A4}$$

O₂ Balance around Annulus # 4

in: $\dot{n}_{D4} y_{L3}$

$\dot{n}_{D4} = 0.90 \dot{n}_{EX3}$

out: $\dot{n}_{G4} y_{B4}$

Accum: $\frac{d(\dot{n}_{B4} y_{B4})}{dt}$

$$\dot{n}_{B4} \frac{dy_{B4}}{dt} + y_{B4} \frac{d\dot{n}_{B4}}{dt} = \dot{n}_{D4} y_{L3} - \dot{n}_{G4} y_{B4} - \alpha_{B4} y_{B4}$$

$$\left[\frac{dy_{B4}}{dt} = \frac{1}{\dot{n}_{B4}} [\dot{n}_{D4} y_{L3} - \dot{n}_{G4} y_{B4} - \alpha_{B4} y_{B4}] \right]$$

$\alpha_{B4} = \dot{n}_{D4} - \dot{n}_{G4}$

$\dot{n}_{G4} = \dot{n}_{D4} - \left(\frac{V_{B4}}{V_{mo}} \right) \alpha$

O₂ Balance around Gap # 4

in: $\dot{n}_{F4} y_{A4} + \dot{n}_{G4} y_{B4}$

out: $\dot{n}_{EX4} y_{C4}$

Accum: $\frac{d(\dot{n}_{C4} y_{C4})}{dt}$

$$\dot{n}_{C4} \frac{dy_{C4}}{dt} + y_{C4} \frac{d\dot{n}_{C4}}{dt} = \dot{n}_{F4} y_{A4} + \dot{n}_{G4} y_{B4} - \dot{n}_{EX4} y_{C4} - \alpha_{C4} y_{C4}$$

$$\left[\frac{dy_{C4}}{dt} = \frac{1}{\dot{n}_{C4}} [\dot{n}_{F4} y_{A4} + \dot{n}_{G4} y_{B4} - \dot{n}_{EX4} y_{C4} - \alpha_{C4} y_{C4}] \right];$$

as before, $\alpha_{C4} = \dot{n}_{F4} + \dot{n}_{G4} - \dot{n}_{EX4}$

O₂ Balance around Scraper Basket

in: $\dot{n}_{ES} y_{C4}$

$\dot{n}_{ES} = 0.20 \dot{n}_{EX4}$

out: $\dot{n}_{FS} y_{A5}$

Accum: $\frac{d(n_{AS} y_{A5})}{dt}$

$$n_{AS} \frac{dy_{A5}}{dt} + y_{A5} \frac{dn_{AS}}{dt} = \dot{n}_{ES} y_{C4} - \dot{n}_{FS} y_{A5}$$

$$\frac{dy_{A5}}{dt} = \frac{1}{n_{AS}} [\dot{n}_{ES} y_{C4} - \dot{n}_{FS} y_{A5} - \alpha_{AS} y_{A5}]$$

$$\alpha_{AS} = \dot{n}_{ES} - \dot{n}_{FS}$$

$$\dot{n}_{FS} = \dot{n}_{ES} - \left(\frac{V_{AS}}{V_{m10}} \right) \alpha$$

O₂ Balance around Annulus # 5

in: $\dot{n}_{DS} y_{C4}$

$\dot{n}_{DS} = 0.80 \dot{n}_{EX4}$

out: $\dot{n}_{GS} y_{B5}$

Accum: $\frac{d(n_{BS} y_{B5})}{dt}$

$$n_{BS} \frac{dy_{B5}}{dt} + y_{B5} \frac{dn_{BS}}{dt} = \dot{n}_{DS} y_{C4} - \dot{n}_{GS} y_{B5}$$

$$\frac{dy_{B5}}{dt} = \frac{1}{n_{BS}} [\dot{n}_{DS} y_{C4} - \dot{n}_{GS} y_{B5} - \alpha_{BS} y_{B5}]$$

$$\alpha_{BS} = \dot{n}_{DS} - \dot{n}_{GS}$$

$$\dot{n}_{GS} = \dot{n}_{DS} - \left(\frac{V_{BS}}{V_{m10}} \right) \alpha$$

O₂ Balance around Gap^{#5}

$$\text{in: } \dot{n}_{F5} y_{A5} + \dot{n}_{G5} y_{B5}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{d(\dot{n}_{C5} y_{C5})}{dt}$$

$$\dot{n}_{C5} \frac{dy_{C5}}{dt} + y_{C5} \frac{d\dot{n}_{C5}}{dt} = \dot{n}_{F5} y_{A5} + \dot{n}_{G5} y_{B5}$$

$$\frac{dy_{C5}}{dt} = \frac{1}{\dot{n}_{C5}} [\dot{n}_{F5} y_{A5} + \dot{n}_{G5} y_{B5} - \dot{n}_{C5} y_{C5}]$$

as before, $\dot{n}_{C5} = \dot{n}_{F5} + \dot{n}_{G5}$

P increase O₂ Balance around Fuel Basket #6

in: $\dot{n}_{E6} y_{CS}$

$$\dot{n}_{E6} = 0.20 \dot{n}_{O2}$$

out: $\dot{n}_{F6} y_{A6}$

Accum: $\frac{d(\dot{n}_{A6} y_{A6})}{dt}$

$$\dot{n}_{A6} \frac{dy_{A6}}{dt} + y_{A6} \frac{d\dot{n}_{A6}}{dt} = \dot{n}_{E6} y_{CS} - \dot{n}_{F6} y_{A6} - \dot{n}_{A6} y_{A6}$$

$$\frac{dy_{A6}}{dt} = \frac{1}{\dot{n}_{A6}} [\dot{n}_{E6} y_{CS} - \dot{n}_{F6} y_{A6} - \dot{n}_{A6} y_{A6}]$$

$$\dot{n}_{A6} = \dot{n}_{E6} - \dot{n}_{F6}$$

$$\dot{n}_{F6} = \dot{n}_{E6} - \left(\frac{V_{A6}}{V_{mco}} \right) \dot{n}_{A6}$$

O₂ Balance around Annulus #6

in: $\dot{n}_{D6} y_{CS}$

out: $\dot{n}_{G1} y_{B6}$

Accum: $\frac{d(\dot{n}_{B6} y_{B6})}{dt}$

$$\dot{n}_{B6} \frac{dy_{B6}}{dt} + y_{B6} \frac{d\dot{n}_{B6}}{dt} = \dot{n}_{D6} y_{CS} - \dot{n}_{G1} y_{B6} - \dot{n}_{B6} y_{B6}$$

$$\therefore \frac{dy_{B6}}{dt} = \frac{1}{\dot{n}_{B6}} [\dot{n}_{D6} y_{CS} - \dot{n}_{G1} y_{B6} - \dot{n}_{B6} y_{B6}]$$

O₂ Balance around Gap #6

$$\text{in: } \dot{n}_{F6} y_{A6} + \dot{n}_{G6} y_{B6}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{d(n_{C6} y_{C6})}{dt}$$

$$n_{C6} \frac{dy_{C6}}{dt} + y_{C6} \frac{dn_{C6}}{dt} = \dot{n}_{F6} y_{A6} + \dot{n}_{G6} y_{B6} - \alpha_{C6} \dot{n}_{C6} y_{C6}$$

$$\frac{dy_{C6}}{dt} = \frac{1}{n_{C6}} [\dot{n}_{F6} y_{A6} + \dot{n}_{G6} y_{B6} - \alpha_{C6} \dot{n}_{C6} y_{C6}]$$

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Air Balance Around FB#1 During Constant Pressure

in: 0

out: $\dot{n}_{F1} y_{A1}$ Accum: $\frac{d(n_{A1} y_{A1})}{dt}$

$$n_{A1} \frac{dy_{A1}}{dt} + y_{A1} \frac{dn_{A1}}{dt} = 0 - \dot{n}_{F1} y_{A1}$$

$$\therefore \frac{dy_{A1}}{dt} = - \frac{\dot{n}_{F1} y_{A1}}{n_{A1}}$$

Air Balance Around Annulus Void

in: 0

out: $\dot{n}_{G1} y_{B1}$ Accum: $\frac{d(n_{B1} y_{B1})}{dt}$

$$n_{B1} \frac{dy_{B1}}{dt} + y_{B1} \frac{dn_{B1}}{dt} = 0 - \dot{n}_{G1} y_{B1}$$

$$\therefore \frac{dy_{B1}}{dt} = - \frac{\dot{n}_{G1} y_{B1}}{n_{B1}}$$

Air Balance Around Gap #1

$$\text{in: } \dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1}$$

$$\text{out: } \dot{n}_{ex1} y_{C1}$$

$$\text{Accum: } \frac{d(n_{C1} y_{C1})}{dt}$$

$$n_{C1} \frac{dy_{C1}}{dt} + y_{C1} \frac{d\dot{n}_{C1}}{dt} = \dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1} - \dot{n}_{ex1} y_{C1}$$

$$\therefore \frac{dy_{C1}}{dt} = \frac{1}{n_{C1}} [\dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1} - \dot{n}_{ex1} y_{C1}]$$

Air Balance Around FB #2

$$\text{in: } \dot{n}_{E2} y_{C1}$$

$$\text{out: } \dot{n}_{F2} y_{A2}$$

$$\text{Accum: } \frac{d(n_{A2} y_{A2})}{dt}$$

$$n_{A2} \frac{dy_{A2}}{dt} + y_{A2} \frac{d\dot{n}_{A2}}{dt} = \dot{n}_{E2} y_{C1} - \dot{n}_{F2} y_{A2}$$

$$\therefore \frac{dy_{A2}}{dt} = \frac{1}{n_{A2}} [\dot{n}_{E2} y_{C1} - \dot{n}_{F2} y_{A2}]$$

Air Balance Around Annulus #2

$$\text{in: } \dot{n}_{D2} y_{C1}$$

$$\text{out: } \dot{n}_{G2} y_{B2}$$

$$\text{Accum: } \frac{d(n_{B2} y_{B2})}{dt}$$

$$n_{B2} \frac{dy_{B2}}{dt} + y_{B2} \frac{d\dot{n}_{B2}}{dt} = \dot{n}_{D2} y_{C1} - \dot{n}_{G2} y_{B2}$$

$$\therefore \frac{dy_{B2}}{dt} = \frac{1}{n_{B2}} [\dot{n}_{D2} y_{C1} - \dot{n}_{G2} y_{B2}]$$

Air Balance Around Gap # 2

$$\text{in: } \dot{n}_{F2} y_{A2} + \dot{n}_{G2} y_{B2}$$

$$\text{out: } \dot{n}_{E2} y_{C2}$$

$$\text{Accum: } \frac{d(n_{C2} y_{C2})}{dt}$$

$$n_{C2} \frac{dy_{C2}}{dt} + y_{C2} \frac{dn_{C2}}{dt} = \dot{n}_{F2} y_{A2} + \dot{n}_{G2} y_{B2} - \dot{n}_{E2} y_{C2}$$

$$\therefore \frac{dy_{C2}}{dt} = \frac{1}{n_{C2}} [\dot{n}_{F2} y_{A2} + \dot{n}_{G2} y_{B2} - \dot{n}_{E2} y_{C2}]$$

Air Balance Around FB # 3

$$\text{in: } \dot{n}_{E3} y_{C2}$$

$$\text{out: } \dot{n}_{F3} y_{A3}$$

$$\text{Accum: } \frac{d(n_{A3} y_{A3})}{dt}$$

Special Case 3 & 7 - constant pressure

Air balance around 2nd FB (w/ bottom SB)

in: $\dot{n}_{F1} y_{A1}$

out: $\dot{n}_{F2} y_{A2}$

Accum: $\frac{d(n_{A2} y_{A2})}{dt}$

$$n_{A2} \frac{dy_{A2}}{dt} + y_{A2} \frac{dn_{A2}}{dt} = \dot{n}_{F1} y_{A1} - \dot{n}_{F2} y_{A2}$$

$$\therefore \frac{dy_{A2}}{dt} = \frac{1}{n_{A2}} [\dot{n}_{F1} y_{A1} - \dot{n}_{F2} y_{A2}]$$

Air balance around 2nd Annulus (w/ bottom SB)

in: $\dot{n}_{G1} y_{B1}$

out: $\dot{n}_{G2} y_{B2}$

Accum: $\frac{d(n_{B2} y_{B2})}{dt}$

$$n_{B2} \frac{dy_{B2}}{dt} + y_{B2} \frac{dn_{B2}}{dt} = \dot{n}_{G1} y_{B1} - \dot{n}_{G2} y_{B2}$$

$$\therefore \frac{dy_{B2}}{dt} = \frac{1}{n_{B2}} [\dot{n}_{G1} y_{B1} - \dot{n}_{G2} y_{B2}]$$

Purge Helium Cycle - changing pressureH₂ Balance around the 1st FBin: $\dot{n}_{H_2}$ out: $\dot{n}_{F1} y_{A1}$ Accum: $\frac{d(n_{A1} y_{A1})}{dt}$

$$n_{A1} \frac{dy_{A1}}{dt} + y_{A1} \frac{dn_{A1}}{dt} = \dot{n}_{H_2} - \dot{n}_{F1} y_{A1}$$

$$\therefore \frac{dy_{A1}}{dt} = \frac{1}{n_{A1}} [\dot{n}_{H_2} - \dot{n}_{F1} y_{A1} - \alpha_{A1} y_{A1}]$$

H₂ Balance around the 1st Annulus

in: 0

out: $\dot{n}_{G1} y_{B1}$ Accum: $\frac{d(n_{B1} y_{B1})}{dt}$

$$n_{B1} \frac{dy_{B1}}{dt} + y_{B1} \frac{dn_{B1}}{dt} = 0 - \dot{n}_{G1} y_{B1}$$

$$\therefore \frac{dy_{B1}}{dt} = -\frac{1}{n_{B1}} [\dot{n}_{G1} y_{B1} + \alpha_{B1} y_{B1}]$$

H₂ Balance around the 1st Gzpin: $\dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1}$ out: $\dot{n}_{EX1} y_{C1}$ Accum: $\frac{d(n_{C1} y_{C1})}{dt}$

$$n_{C1} \frac{dy_{C1}}{dt} + y_{C1} \frac{dn_{C1}}{dt} = \dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1} - \dot{n}_{EX1} y_{C1}$$

$$\therefore \frac{dy_{C1}}{dt} = \frac{1}{n_{C1}} [\dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1} - \dot{n}_{EX1} y_{C1} - \alpha_{C1} y_{C1}]$$

H₂ Balance Around the 2nd FB - changing pressure

$$\text{in: } \dot{n}_{H_2} + \dot{n}_{E2} y_{E1}$$

$$\text{out: } \dot{n}_{F2} y_{F2}$$

$$\text{Accum: } \frac{d(n_{A2} y_{A2})}{dt}$$

$$n_{A2} \frac{dy_{A2}}{dt} + y_{A2} \frac{dn_{A2}}{dt} = \dot{n}_{H_2} + \dot{n}_{E2} y_{E1} - \dot{n}_{F2} y_{F2}$$

$$\frac{dy_{A2}}{dt} = \frac{1}{n_{A2}} [\dot{n}_{H_2} + \dot{n}_{E2} y_{E1} - \dot{n}_{F2} y_{F2} - \alpha_{A2} y_{A2}]$$

for FB's above #1 $\rightarrow \therefore \frac{dy_{Ai}}{dt} = \frac{1}{n_{Ai}} [\dot{n}_{H_2} + \dot{n}_{Ei} y_{E(i-1)} - \dot{n}_{Fi} y_{Fi} - \alpha_{Ai} y_{Ai}]$

$$i = 2-5 \text{ or } i = 2-6 \text{ (w/ 6 FB's)}$$

H₂ Balance Around 2nd Annulus

$$\text{in: } \dot{n}_{B2} y_{B1}$$

$$\text{out: } \dot{n}_{B2} y_{B2}$$

$$\text{Accum: } \frac{d(n_{B2} y_{B2})}{dt}$$

$$n_{B2} \frac{dy_{B2}}{dt} + y_{B2} \frac{dn_{B2}}{dt} = \dot{n}_{B2} y_{B1} - \dot{n}_{B2} y_{B2}$$

$$\frac{dy_{B2}}{dt} = \frac{1}{n_{B2}} [\dot{n}_{B2} y_{B1} - \dot{n}_{B2} y_{B2} - \alpha_{B2} y_{B2}]$$

for Annulus above 1 $\rightarrow \therefore \frac{dy_{Bi}}{dt} = \frac{1}{n_{Bi}} [\dot{n}_{Bi} y_{B(i-1)} - \dot{n}_{Bi} y_{Bi} - \alpha_{Bi} y_{Bi}]$

$$i = 2-5 \text{ or } i = 2-6 \text{ (w/ 6 FB's)}$$

H₂ Balance Around 2nd Gap

$$\text{in: } \dot{n}_{F2} y_{A2} + \dot{n}_{G2} y_{B2}$$

$$\text{out: } \dot{n}_{ex2} y_{c2}$$

$$\text{Accum: } \frac{d(n_{c2} y_{c2})}{dt}$$

$$n_{c2} \frac{dy_{c2}}{dt} + y_{c2} \frac{dn_{c2}}{dt} = \dot{n}_{F2} y_{A2} + \dot{n}_{G2} y_{B2} - \dot{n}_{ex2} y_{c2}$$

$$\frac{dy_{c2}}{dt} = \frac{1}{n_{c2}} [\dot{n}_{F2} y_{A2} + \dot{n}_{G2} y_{B2} - \dot{n}_{ex2} y_{c2} - \alpha_{c2} y_{c2}]$$

$$\text{for } i = 1-4 \quad \text{for } 5 \text{ FB's}$$

$$\text{or}$$

$$\text{for } i = 1-5 \quad \text{for } 6 \text{ FB's}$$

for
Gaps
except top

$$\rightarrow \frac{dy_{ci}}{dt} = \frac{1}{n_{ci}} [\dot{n}_{Fi} y_{Ai} + \dot{n}_{Gi} y_{Bi} - \dot{n}_{exi} y_{ci} - \alpha_{ci} y_{ci}]$$

Top Gap Space H₂ Balance - changing pressure

j = 5 or 6

$$\text{in: } \dot{n}_{Fj} y_{Aj} + \dot{n}_{Gj} y_{Bj}$$

$$\text{out: } 0$$

$$\text{Accum: } \frac{d(n_{cj} y_{cj})}{dt}$$

$$n_{cj} \frac{dy_{cj}}{dt} + y_{cj} \frac{dn_{cj}}{dt} = \dot{n}_{Fj} y_{Aj} + \dot{n}_{Gj} y_{Bj}$$

j=5
w/5 FB's

$$\frac{dy_{c5}}{dt} = \frac{1}{n_{c5}} [\dot{n}_{F5} y_{A5} + \dot{n}_{G5} y_{B5} - \alpha_{c5} y_{c5}]$$

and
j=6
w/6 FB's

$$\frac{dy_{c6}}{dt} = \frac{1}{n_{c6}} [\dot{n}_{F6} y_{A6} + \dot{n}_{G6} y_{B6} - \alpha_{c6} y_{c6}]$$

charging
pressureH₂ Balance Around 2nd F.B (w/ bottom SB)

$$\text{in: } \dot{n}_{F1} y_{A1} + \dot{n}_{H2}$$

$$\text{out: } \dot{n}_{F2} y_{A2}$$

$$\text{Accum: } \frac{d(n_{A2} y_{A2})}{dt}$$

$$n_{A2} \frac{dy_{A2}}{dt} + y_{A2} \frac{dn_{A2}}{dt} = \dot{n}_{F1} y_{A1} + \dot{n}_{H2} - \dot{n}_{F2} y_{A2} - \alpha_{A2} y_{A2}$$

$$\therefore \frac{dy_{A2}}{dt} = \frac{1}{n_{A2}} [\dot{n}_{F1} y_{A1} + \dot{n}_{H2} - \dot{n}_{F2} y_{A2} - \alpha_{A2} y_{A2}]$$

H₂ Balance Around 2nd Annulus (w/ bottom SB)

$$\text{in: } \dot{n}_{G1} y_{B1}$$

$$\text{out: } \dot{n}_{G2} y_{B2}$$

$$\text{Accum: } \frac{d(n_{B2} y_{B2})}{dt}$$

$$n_{B2} \frac{dy_{B2}}{dt} + y_{B2} \frac{dn_{B2}}{dt} = \dot{n}_{G1} y_{B1} - \dot{n}_{G2} y_{B2} - \alpha_{B2} y_{B2}$$

$$\therefore \frac{dy_{B2}}{dt} = \frac{1}{n_{B2}} [\dot{n}_{G1} y_{B1} - \dot{n}_{G2} y_{B2} - \alpha_{B2} y_{B2}]$$

Purge Helium Cycle - constant Pressure
H₂ Balance around the 1st FB

in: $\dot{n}_{H_2}$

out: $\dot{n}_{F1} y_{A1}$

Accum: $\frac{d(n_{A1} y_{A1})}{dt}$

$$n_{A1} \frac{dy_{A1}}{dt} + y_{A1} \frac{dn_{A1}}{dt} = \dot{n}_{H_2} - \dot{n}_{F1} y_{A1}$$

$$\frac{dy_{A1}}{dt} = \frac{1}{n_{A1}} [\dot{n}_{H_2} - \dot{n}_{F1} y_{A1}]$$

H₂ Balance around the 1st Annulus

in: 0

out: $\dot{n}_{G1} y_{B1}$

Accum: $\frac{d(n_{B1} y_{B1})}{dt}$

$$n_{B1} \frac{dy_{B1}}{dt} + y_{B1} \frac{dn_{B1}}{dt} = 0 - \dot{n}_{G1} y_{B1}$$

$$\therefore \frac{dy_{B1}}{dt} = -\frac{\dot{n}_{G1} y_{B1}}{n_{B1}}$$

H₂ Balance around the 1st Gap

in: $\dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1}$

out: $\dot{n}_{EX1} y_{C1}$

Accum: $\frac{d(n_{C1} y_{C1})}{dt}$

$$n_{C1} \frac{dy_{C1}}{dt} + y_{C1} \frac{dn_{C1}}{dt} = \dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1} - \dot{n}_{EX1} y_{C1}$$

$$\frac{dy_{C1}}{dt} = \frac{1}{n_{C1}} [\dot{n}_{F1} y_{A1} + \dot{n}_{G1} y_{B1} - \dot{n}_{EX1} y_{C1}]$$

For FB's $\bar{i} = 2-5$ or $\bar{i} = 2-6$

at constant Pressure, (omitting α_{Ai} term)

$$\frac{dy_{Ai}}{dt} = \frac{1}{n_{Ai}} [\dot{n}_{H_2} + \dot{n}_{Ei} y_{L(\bar{i}-1)} - \dot{n}_{Fi} y_{Ai}]$$

For Annulus $\bar{i} = 2-5$ or $\bar{i} = 2-6$

at constant Pressure, (omitting α_{Bi} term)

$$\frac{dy_{Bi}}{dt} = \frac{1}{n_{Bi}} [\dot{n}_{D\bar{i}} y_{E(\bar{i}-1)} - \dot{n}_{G\bar{i}} y_{B\bar{i}}]$$

For Gap $\bar{i} = 1-5$ or $\bar{i} = 1-6$

at constant Pressure, (omitting α_{Ci} term)

$$\frac{dy_{Ci}}{dt} = \frac{1}{n_{Ci}} [\dot{n}_{Fi} y_{Ai} + \dot{n}_{Gi} y_{Bi} - \dot{n}_{Exi} y_{Ci}]$$

SPECIAL CASE 3 ml 7Constant PressureH₂ Balance Around 2ND FB (w/bottom SB)omitting α_{02} term,

$$\therefore \frac{dy_{02}}{dt} = \frac{1}{n_{02}} [\dot{n}_{01} y_{01} + \dot{n}_{02} - \dot{n}_{02} y_{02}]$$

H₂ Balance Around 2ND Annulus (w/bottom SB)omitting α_{02} term,

$$\frac{dy_{02}}{dt} = \frac{1}{n_{02}} [\dot{n}_{01} y_{01} - \dot{n}_{02} y_{02}]$$

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Special Case 3 & 7 - changing pressure

Air balance around 2nd FB (w/ bottom SB)

in: $\dot{n}_F y_{A1}$

out: $\dot{n}_F y_{A2}$

Accum: $\frac{d(n_{A2} y_{A2})}{dt}$

$$n_{A2} \frac{dy_{A2}}{dt} + y_{A2} \frac{dn_{A2}}{dt} = \dot{n}_F y_{A1} - \dot{n}_F y_{A2} - \alpha_{A2} y_{A2}$$

$$\frac{dy_{A2}}{dt} = \frac{1}{n_{A2}} [\dot{n}_F y_{A1} - \dot{n}_F y_{A2} - \alpha_{A2} y_{A2}]$$

Air Balance around 2nd Annulus (w/ bottom SB)

in: $\dot{n}_G y_{G1}$

out: $\dot{n}_G y_{G2}$

Accum: $\frac{d(n_{G2} y_{G2})}{dt}$

$$n_{G2} \frac{dy_{G2}}{dt} + y_{G2} \frac{dn_{G2}}{dt} = \dot{n}_G y_{G1} - \dot{n}_G y_{G2} - \alpha_{G2} y_{G2}$$

$$\therefore \frac{dy_{G2}}{dt} = \frac{1}{n_{G2}} [\dot{n}_G y_{G1} - \dot{n}_G y_{G2} - \alpha_{G2} y_{G2}]$$