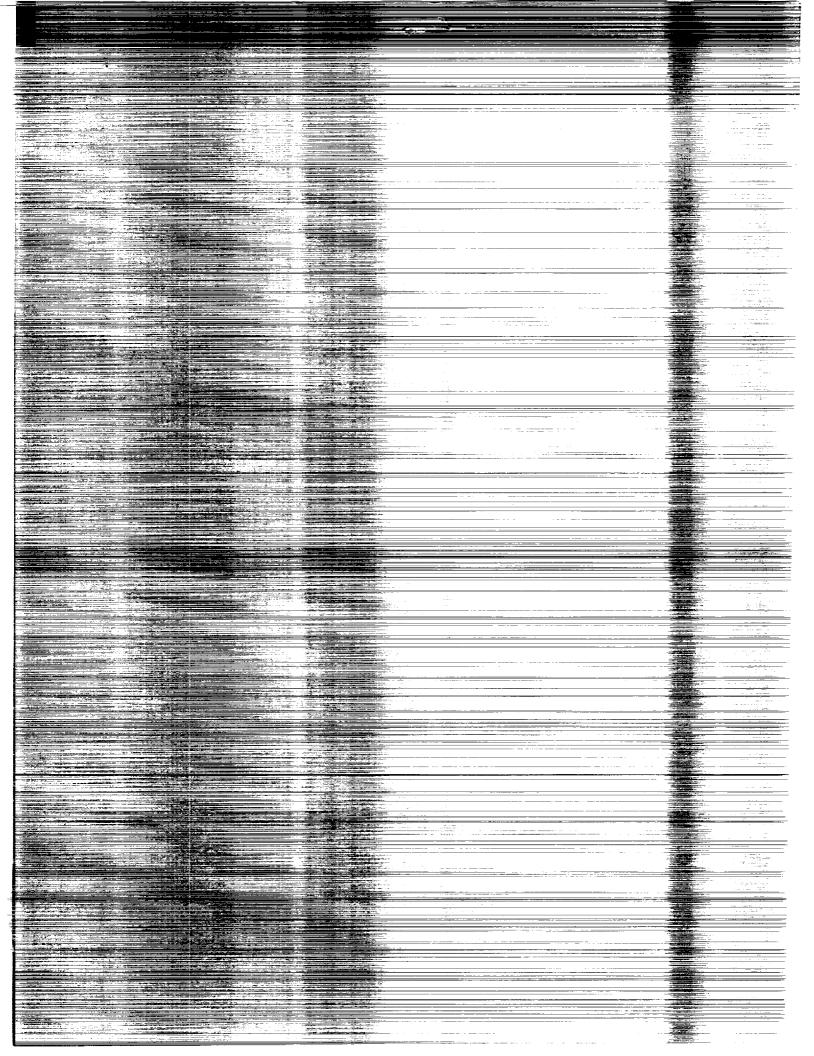
NASA Technical Memorandum 4202

Space Station Freedom Environmental
Control and Life Support System
(ECLSS) Phase III Simplified
Integrated Test Trace Contaminant
Control Subsystem Performance

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Space Station Freedom Environmental Control and Life Support System (ECLSS) Phase III Simplified Integrated Test Trace Contaminant Control Subsystem Performance

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TECHNICAL MEMORANDUM

SPACE STATION FREEDOM ECLSS PHASE III SIMPLIFIED INTEGRATED TEST TRACE CONTAMINANT CONTROL SUBSYSTEM PERFORMANCE

INTRODUCTION

Since 1986, phased testing of the Space Station Freedom (S.S. Freedom) environmental control and life support system (ECLSS) has been conducted in a test facility, the Core Module Integration Facility (CMIF), located at the Marshall Space Flight Center. The test phases consist of subsystem tests and system tests which integrate several ECLSS subsystems for testing. Phase I testing encompasses all subsystem tests required for subsystem characterization and checkout to qualify the subsystem for integrated testing. Phases II and III are integrated system tests of the ECLSS air revitalization subsystems.

Air revitalization tests during Phase II tested the performance of carbon dioxide removal, carbon dioxide reduction, oxygen generation, and trace contaminant control subsystems in an integrated configuration. The Phase III simplified integrated test (SIT) conducted from July 30, 1989, through August 11, 1989, expanded on the Phase II testing by substituting the Bosch carbon dioxide reduction process (BCRS) for the Sabatier carbon dioxide reduction process (SCRS). In addition, the trace contaminant control subsystem (TCCS) was integrated directly with other air revitalization subsystems. This provided a rigorous test of the TCCS for controlling process bleed streams produced by other ECLSS subsystems and provided important information on the S.S. Freedom air revitalization system (ARS) configuration. Figure 1 shows a simplified process flow diagram of the major SIT subsystems [1].

The interface between the TCCS and the BCRS is of particular interest to the overall air quality in the S.S. Freedom. BCRS bleed products include methane, carbon monoxide, hydrogen, carbon dioxide, oxygen, and water vapor. Of particular interest are the methane, hydrogen, and carbon monoxide components since they provide a rigorous test of the TCCS high temperature catalytic oxidizer subsassembly performance and they are major atmospheric constituents monitored in the S.S. Freedom on a regular basis. The ability of the TCCS to control these bleed components gives a good indication of its ability to control these and other airborne contaminants controlled primarily by catalytic oxidation. In addition, since the TCCS had not been directly integrated with other ECLSS subsystems during past tests, it is an increase in the level of complexity of TCCS testing.

Past TCCS tests focused primarily on subsystem characterization testing with tests designed to assess individual subassembly performance. These tests provided data to verify the TCCS design parameters such as subassembly sizing and performance under varying flow conditions. Further subsystem tests focused on several air contaminants of interest to assess the overall subsystem performance when exposed to these potential spacecraft contaminants. Additional contamination loads from subsystem bleeds and purges were not considered during these earlier tests. As the S.S.

Freedom air revitalization system design progressed, the TCCS was identified as a powerful contamination control device, particularly if bleed and purge streams could be directly interfaced with it and processed before entering the cabin. Analysis supported the interface concept but the actual impact of these interfaces on the TCCS performance were virtually unknown. The Phase III SIT represents the first direct integration of the TCCS with other subsystem bleed streams and an attempt to confirm past performance analyses and data [2].

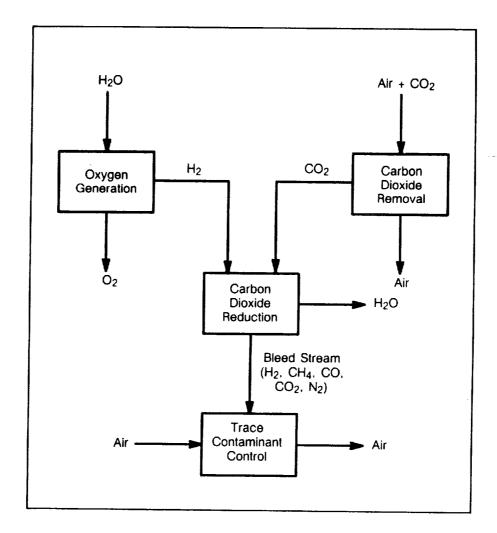


Figure 1. SIT subsystem interfaces.

SUBSYSTEM DESCRIPTION

The TCCS removes gas phase trace contaminants from a spacecraft atmosphere by circulating air through a series of packed sorbent beds and a high temperature catalytic oxidizer. Located in either a high flow or low flow branch of the TCCS, each trace contaminant removal subassembly targets a range of contaminants to provide an efficient contamination control approach. Table 1 details some subassembly features while Figure 2 illustrates the location of each subassembly in the TCCS.

Table 1. TCCS subassembly characteristics.

COMPONENT	FLOW (m³/s)	LENGTH (m)	DIAMETER (m)	ΔP (Pa)	MASS (kg)
Fixed Bed	0.0165	0.381	0.330	623	30.4
Presorbent Bed	0.00212	0.152	0.127	237	1.59
Postsorbent Bed	0.00212	0.222	0.127	386	2.04
Catalytic Oxidizer	0.00212	0.0914	0.0558	1490	14.1
Axial Fan (11500 RPM/55W)	0.0165	0.146	0.114	672	1.35
Centrifugal Blower (22500 RPM/90W)	0.00423			4230	1.02

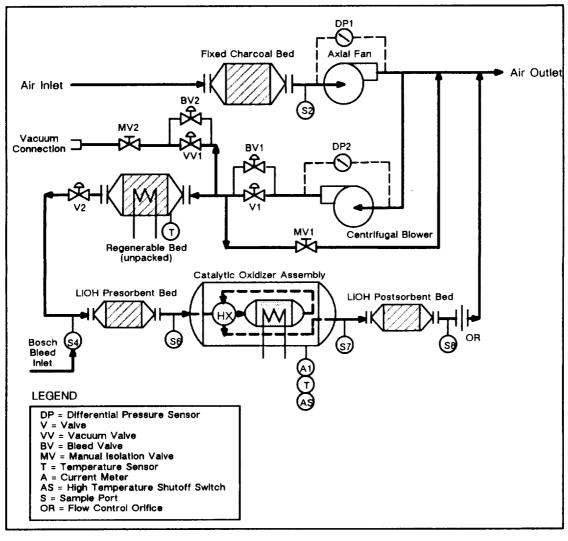


Figure 2. Trace contaminant control subsystem.

High Flow Branch

The high flow branch consists of a vane axial fan which draws 0.0113 m³/s (24 ft³/min) through a fixed charcoal bed. The charcoal bed contains 21.8 kg (48 lbm) of phosphoric acid-impregnated activated carbon. This bed functions as a removal device for high molar volume contaminants and ammonia [2].

Low Flow Branch

Approximately 0.00151 m³/s (3.2 ft³/min) of the high flow branch is drawn into the low flow branch by a centrifugal blower, processed, and mixed with the air in the high flow branch before exhausting to the test chamber atmosphere. This branch contains a regenerable charcoal bed, a lithium hydroxide (LiOH) presorbent bed, a high temperature catalytic oxidizer, and a LiOH postsorbent bed. The regenerable bed was operated empty since the present S.S. Freedom TCCS design concept does not include a regenerable bed. If it was operated with the regenerable bed, the bed's function is to remove low molar volume contaminants. The presorbent bed contains 0.91 kg (2.0 lbm) of LiOH sorbent which removes acidic gases and potential catalyst poisons from the air before it enters the catalytic oxidizer. The catalytic oxidizer then oxidizes any contaminants which have not been removed by the fixed charcoal bed and presorbent beds. This assembly consists of a five-pass cross-counter flow plate fin heat exchanger and an electrically-heated catalyst canister. Air enters the heat exchanger where it is preheated by exiting air. The air is heated to the final operating temperature by two 70-W electric heaters located in the catalyst canister. Heated air flows through a bed of 0.5 percent palladium on 3.175 mm (0.125 in) diameter alumina (Al₂O₃) spheres. Contaminants which are not easily removed by the preceding removal assemblies are oxidized in the canister. Air, containing oxidation products, flows out of the catalytic oxidizer assembly and into a LiOH postsorbent bed which contains 1.36 kg (3 lbm) of LiOH. The oxidation products are removed in this bed and clean air flows back to the high flow branch and then exhausts to the cabin atmosphere [2].

TEST CONFIGURATION

Subsystem Interfaces

The SIT is the first time that the TCCS has been integrated with other ECLSS ARS subsystems. The air inlet to the fixed charcoal bed was interfaced with the temperature and humidity control system. This interface reduced the relative humidity of the inlet air to enhance contaminant removal and avoid contaminant displacement by water vapor. The major interface was with the BCRS. The Bosch process produces a bleed stream of reactants, inerts, and reaction products such as methane, carbon monoxide, hydrogen, nitrogen, oxygen, and carbon dioxide. Methane, carbon monoxide, and hydrogen are particularly important since they are major atmosphere constituents generated from material offgassing and crew metabolic processes. The bleed stream was introduced through a port just before the presorbent bed to obtain optimum oxidation of these contaminants. The TCCS exhaust was interfaced directly with the test chamber atmosphere.

Since the SIT was the first time that the TCCS and BCRS bleed streams were integrated, several precautions were taken to ensure that safety hazards resulting from toxic and combustible gas mixtures were minimized. A pretest analysis, documented in Appendix A, was conducted to determine the best location for the BCRS bleed stream interface and to determine the TCCS performance conditions which could result in a flammable gas mixture in the TCCS. This analysis indicated that introducing the bleed stream just before the fixed carbon bed would result in a toxic buildup of carbon monoxide in a closed test chamber, but introducing the bleed stream before the LiOH presorbent bed provided more complete carbon monoxide control. Also methane and hydrogen concentrations would be controlled more effectively. The analysis showed that a BCRS bleed stream up to 0.0000167 m³/s (0.035 ft³/min) resulted in methane and hydrogen concentrations of 0.86 volume percent and 0.35 volume percent, respectively, when mixed with a 0.00165 m³/s (3.5 ft³/min) TCCS air flow. This is below the lower flammability limits of 5 volume percent for methane and 4 volume percent for hydrogen. As a precaution, the BCRS bleed stream was diverted from the TCCS if the TCCS low flow branch flowrate fell below 0.000472 m³/s (1 ft³/min) [3].

Instrumentation

TCCS instrumentation provides simple subsystem status information on electrical current, differential pressure, and catalytic oxidizer temperature. Table 2 documents the major instrumentation measurements and their nominal values. Differential pressure measurements are taken across the axial fan and centrifugal blower to determine whether they are operating properly. Most of the other data provided relates to the catalytic oxidizer operating conditions. The catalytic oxidizer heater current is monitored and is used as a control input to an overcurrent cutoff switch which shutsdown the heater current in the event of a power surge. Likewise, the catalytic oxidizer temperature is monitored by a thermocouple probe which monitors the catalytic oxidizer external canister temperature. This temperature reading also serves as a control input for an overtemperature cutoff switch which shutsdown the heater current. The temperature limit is required to protect the catalyst from extremely high temperatures which may result in its thermal degradation. A flow measurement was added in the low flow branch to aid in conducting mass and energy balances on the catalytic oxizider assembly. Figure 1 shows the location of the major instrument readings.

Table 2. TCCS process measurements.

MEASUREMENT	TEST ID NUMBER	UNITS	NOMINAL VALUE
Catalyic Oxidizer Heater Current	JI01	Amps	1.3
Catalyic Oxidizer canister Temp	JT01	Fahrenheit	680
Centrifugal Blower Differential Pressure	JP01	in. H₂O	17
Axial Fan Differential Pressure	JP02	in. H₂O	3.5
Low Flow Branch Flow Rate	JF01	ft³/min	3.2

SUBSYSTEM PERFORMANCE

Expected Performance

Design literature for the TCCS shows that the subsystem should operate at 0.0165 m³/s (35 ft³/min) in the high flow branch and 0.00201 m³/s (4.25 ft³/min) in the low flow branch. These flow rates produce a pressure drop of 672 Pa (0.097 psi) and 4,230 Pa (0.61 psi) across the vane axial fan and centrifugal blower, respectively. The catalytic oxidizer external canister temperature reaches 615 K (650 °F) which corresponds to an air temperature of 672 K (750 °F). Figure 3 shows the expected catalytic oxidizer operating point. At this temperature approximately 9 percent of the methane and 100 percent of the carbon monoxide and hydrogen will be oxidized per pass.

Test Performance

The TCCS performance during the SIT exceeded the expected performance for methane oxidation, 67.3 percent per pass, but fell short of expectations for carbon monoxide oxidation which achieved an apparent 83.1 percent per pass. Sample analysis results illustrating these efficiencies are summarized in Table 3. The increase in methane conversion was accompanied by

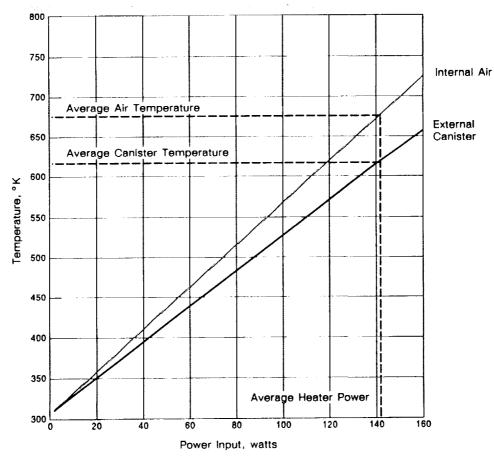


Figure 3. Catalytic oxidizer performance at 7.13 m³/h air flowrate.

Table 3. Summary of TCCS air sample analysis results.

SAMPLE IDENTIFICATION	CAT. OXIDIZER CONCENTRATION SAMPLE LOCATION		CONV	ERSION		
NUMBER	Inlet	Outlet	CH₄	CO	CH₄	CO
JS6-EH-0935-[8-3-89] * JS7-EH-0945-[8-3-89] *	Х	×	30.21 ppm 0.00 ppm	0.00 ppm 0.00 ppm	-	-
JS6-EH-1102-[8-3-89] JS7-EH-1105-[8-3-89]	х	×	4543.9 ppm 956.1 ppm	171.6 ppm 26.1 ppm	0.790	0.848
JS6-BAC-0657-[8-4-89] JS7-BAC-0659-[8-4-89]	Х	×	0.13 vol% 0.05 vol%	<0.2 vol% <0.2 vol%	0.615	-
JS6-BAC-1232-[8-4-89] JS7-BAC-1236-[8-4-89]	Х	×	0.17 vol% 0.04 vol%	<0.2 vol% <0.2 vol%	0.765	-
JS6-EH-1632-[8-4-89] JS7-EH-1642-[8-4-89]	Х	×	3204.13 ppm 694.59 ppm	147.12 ppm 24.28 ppm	0.783	0.835
JS6-EH-0818-[8-5-89] JS7-EH-0826-[8-5-89]	Х	×	2693.05 ppm 835.23 ppm	135.46 ppm 23.18 ppm	0.690	0.829
JS6-BAC-1524-[8-7-89] JS7-BAC-1525-[8-7-89]	×	x	0.16 vol% 0.07 vol%	<0.2 vol% <0.2 vol%	0.562	-
JS6-BAC-1734-[8-8-89] * JS7-BAC-1737-[8-8-89] *	х	x	<0.4 vol% <0.4 vol%	<0.2 vol% <0.2 vol%	-	-
JS6-EH-1057-[8-10-89] JS7-EH-1101-[8-10-89]	×	x	2735.94 ppm 470.10 ppm	141.35 ppm 26.44 ppm	0.828	0.813
JS6-EH-0915-[7-31-89] JS7-EH-0919-[7-31-89]	×	х	25.0 ppm 16.2 ppm	-	0.352	_
AVERAGE CONVERSION					0.673	0.831

^{*} Background samples not included in performance evaluation.

an increase in the catalytic oxidizer operating temperature which resulted from the energy released by the exothermic oxidation reactions taking place in the reactor. The external canister temperature averaged 633 K (710 °F) during the time the TCCS was integrated with the BCRS. This corresponds to an air temperature of 711 K (820 °F). Figure 4 shows the actual catalytic oxidizer operating point. Differential pressures for both the axial fan and centrifugal blower were low, having values of 610 Pa (0.088 psi) and 4,110 Pa (0.596 psi), respectively. The lower differential pressure reading for the centrifugal blower was accompanied by a low flow branch flow rate which averaged 0.00151 m³/s (3.2 ft³/min). This flow rate is lower than expected but is consistent with the lower blower differential pressure.



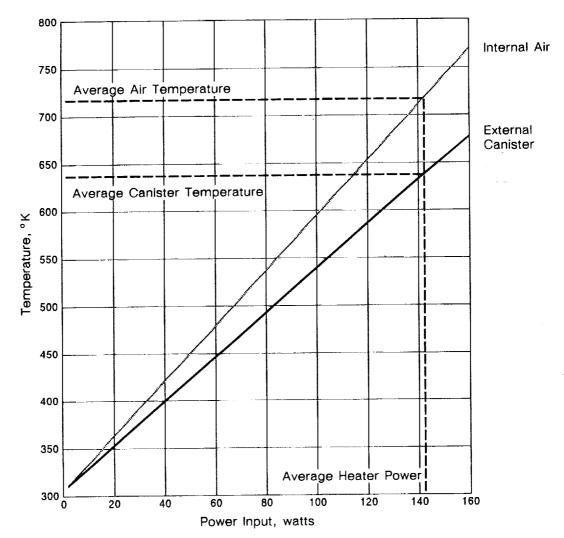


Figure 4. Actual catalytic oxidizer performance at 5.44 m³/h air flowrate.

DISCUSSION OF RESULTS

Contaminant Oxidation Efficiency

Contaminants introduced into the TCCS through the BCRS bleed stream are an excellent performance challenge for the TCCS catalytic oxidizer assembly. The contaminants of interest are methane, carbon monoxide, and hydrogen. Expected oxidation efficiencies for these contaminants are 9 percent for methane and 100 percent for both carbon monoxide and hydrogen. Analytical results of gas samples taken of the catalytic oxidizer assembly influent and effluent, shown in Table 3, show an average oxidation efficiency of 67.3 percent for methane and 83.1 percent for carbon monoxide. Hydrogen oxidation efficiency could not be determined from the sample analysis because the inlet and outlet concentrations fell below the analytical instrument's sensitivity.

Improved methane oxidation efficiency was obtained because the catalytic oxidizer temperature was much higher than expected. Figure 5 shows the expected and actual methane oxidation

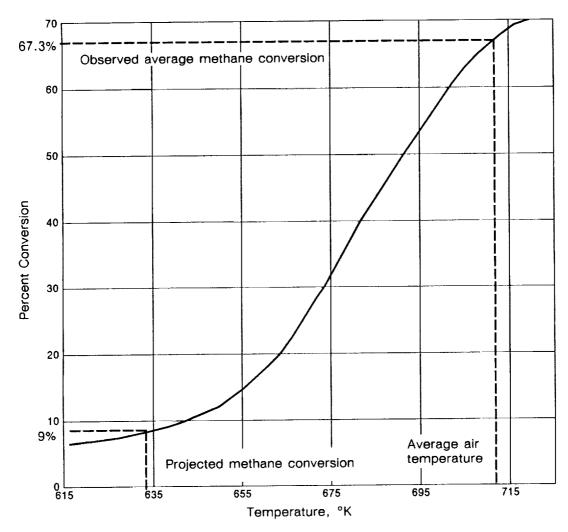


Figure 5. Catalytic oxidizer methane conversion performance.

efficiencies as a function of operating temperature. The average temperature of 711 K ($820~^\circ F$) corresponds directly to 67.3 percent methane conversion.

Poor carbon monoxide oxidation efficiency was not expected. Design literature shows that carbon monoxide oxidation efficiency is 100 percent per pass at these operating conditions. The temperature experienced during the SIT should not result in poor conversion. However, mass balances conducted during post-test analysis supports the observed oxidation efficiency. This analysis, documented in Appendix B, considers two cases for carbon monoxide oxidation. The first case assumes that 83.1 percent of the carbon monoxide fed to the catalytic oxidizer is oxidized while the second case assumes 100 percent oxidation of the feed carbon monoxide and 93 percent oxidation of carbon monoxide produced by incomplete oxidation of methane within the reactor. Both cases support the test results; however, the case which assumes incomplete methane oxidation is considered the more likely mechanism when past carbon monoxide oxidation performance results are considered. The second case also indicates that the carbon monoxide oxidation is a function of the catalytic oxidizer residence time. Additional testing will be required to determine the mechanism of this result.

Predicted Test Chamber Concentration

Post-test analysis, shown in Figure 6, predicting the subsystem's capability to control contaminant concentrations to levels below the spacecraft maximum allowable concentration (SMAC) indicates that the conditions of the SIT would result in a methane concentration at 23 percent of its SMAC of 1,771 mg/m³ and a carbon monoxide concentration at 76 percent of its SMAC of 28.60 mg/m³ in a closed test chamber at the end of the SIT.

The conditions experienced during the SIT represent a worst case for BCRS bleed stream composition and flow rate. An impure carbon dioxide stream was delivered to the BCRS resulting in a buildup of inerts in the reactor and a corresponding high bleed stream flow containing a large amount of reactants, reaction intermediates, and reaction products. The results obtained from TCCS air samples at the high temperature catalytic oxidizer inlet and outlet indicate an apparent carbon monoxide oxidation efficiency of 83.1 percent per pass. This efficiency was expected to be 100 percent. If the expected efficiency had been achieved, the projected carbon monoxide concentration in a closed test chamber would be virtually zero. Additional testing will be required to investigate the carbon monoxide removal results obtained in the SIT and the potential for carbon monoxide production from incomplete hydrocarbon oxidation within the TCCS catalytic oxidizer.

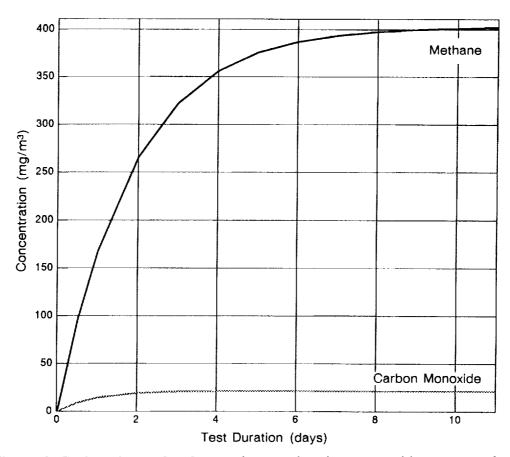


Figure 6. Projected test chamber methane and carbon monoxide concentrations.

Catalytic Oxidizer Temperature

During the SIT, the catalytic oxidizer operated at much higher temperatures than expected. After achieving integration with the BCRS bleed stream, the external canister temperature rose to as high as 700 K (800 °F) which corresponds to an air temperature of 755 K (900 °F). The average external canister temperature was 650 K (710 °F) which corresponds to an air temperature of 711 K (820 °F). This temperature rise results from the additional energy released by the exothermic oxidation reactions occurring in the catalytic oxidizer canister. A post-test analysis of the energy released during these reactions predicts an air temperature of 703 K (806 °F) if the design temperature of 633 K (680 °F) is reached. This analysis is documented in Appendix C. It must be noted that the analysis assumes energy losses through conduction and radiation routes are minimal.

The high temperatures experienced during the SIT required some precautions to protect the catalyst from thermal degradation. Temperatures above 811 K (1,000 °F) may cause thermal degradation of the catalyst resulting in reduced oxidation efficiencies. Since the TCCS flow rate in the low flow branch is controlled by a fixed orifice plate, the temperature in the catalytic oxidizer could not be regulated by controlling the flow rate. Therefore, when the temperature approached 755 K (900 °F), the BCRS bleed stream was diverted to an external duct for a period of time to allow the catalytic oxidizer to cool. This technique is not desirable, especially when the BCRS bleed is continuous and must interface with the TCCS in an uninterrupted manner to achieve efficient contamination control. Modifications to the predevelopment TCCS to allow flow rate regulation will eliminate the need to deintegrate the BCRS bleed stream from the TCCS in future testing.

TEST ANOMALIES

The TCCS operated with few complications during the entire test. The major adjustment made during the test was to integrate and deintegrate the TCCS and BCRS bleed stream as necessary. Minor adjustments were required for the catalytic oxidizer thermocouple probe which provides temperature readings since it vibrated loose from its contact point and required reseating periodically. These anomalies will be corrected by modifying the predevelopment TCCS to provide fair flowrate control and consistent temperature data.

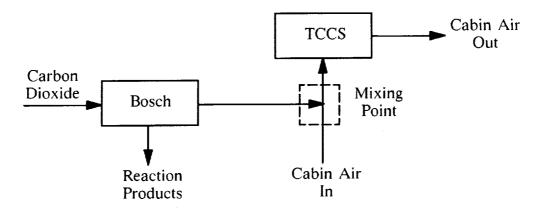
CONCLUSIONS AND RECOMMENDATIONS

The SIT demonstrated that the TCCS can be successfully integrated with other ECLSS ARS subsystems and can operate continously for extended periods of time with minimal adjustment. The oxidation efficiencies obtained in the test indicate that TCCS performance is sensitive to ARS interfaces. Additional testing is required to understand and validate the TCCS removal capabilities for methane and carbon monoxide produced by ARS subsystems. Efficiency sensitivity to air flow rate, catalytic oxidizer temperature, and bleed stream composition should be investigated in future TCCS development tests to further characterize TCCS performance under varying ARS operating conditions. These tests would provide data necessary to optimizing TCCS interfaces with ARS subsystems and lead to an efficient S.S. Freedom TCCS design.

APPENDIX A

TCCS/BCRS Bleed Interface Safety Analysis

SAFETY ANALYSIS OF THE TCCS/BOSCH INTERFACE



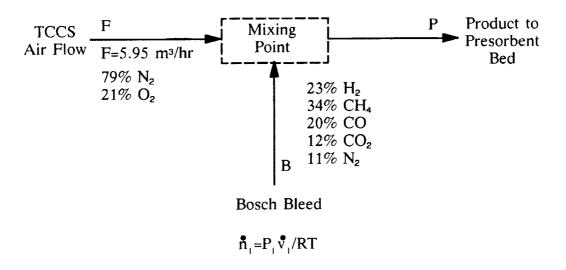
Mixing Point: T=298 K P=1 atm

Hydrogen and Methane Flammability Data: (CH₄ and H₂ in air at 298 K and 1 atm)

SPECIES	LOWER FLAMMABILITY LIMIT (% vol)	UPPER FLAMMABILITY LIMIT (% vol)	SPONTANEOUS IGNITION TEMPERATURE (°C)
H ₂	4.0 (1)	75.0 (1)	571.1 (4)
CH4	5.4 (1) 5.0 (2) 5.3 (3) 4.35 (4)	15.0 (1) 15.0 (2) 15.0 (3) 15.53 (4)	632.2 (4)

References:

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- 2. Flammability Characteristics of Combustible Gases and Vapors. U. S. Dept. of the Interior. Bureau of Mines; 1965.
- 3. Lewis, B.; von Elbe, G. Combustion, Flames, and Explosions of Gases, Third Edition. New York: Academic Press, Inc.; 1987.
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CASE 1: BOSCH BLEED = 500 cm³/min

F=5.95 m³/hr Nitrogen mass flow=5,384,707.3 mg/hr Oxygen mass flow=1,635,016.6 mg/hr

Overall Mass Balance:

SPECIES	F (mg/hr) +	B (mg/hr) =	P (mg/hr)	n (mol/hr)	y,
N ₂	5,384,707.3	6,544.8	5,391,252.1	192.40	0.784
O ₂	1,635,016.6	0.0	1,635,016.6	51.10	0.208
CH4	0.0	11,585.4	11,585.4	0.72	0.003
H ₂	0.0	984.6	984.6	0.49	0.002
СО	0.0	11,898.6	11,898.6	0.42	0.002
CO ₂	0.0	11,217.0	11,217.0	0.25	0.001
TOTALS				245.38	1.000

CASE 2: BOSCH BLEED = 1000 cm³/min with a high methane and hydrogen content

$$\mathbf{n}_1 = \mathbf{y}_1 \mathbf{v}_1 \mathbf{P}/\mathbf{R}\mathbf{T}$$

P=1.837 atm T=316 K

 $F=5.95 \text{ m}^3/\text{hr}$

Nitrogen mass flow=5,384,707.3 mg/hr

Oxygen mass flow=1,635,016.6 mg/hr

B=1000 cm³/min

50% methane

20% oxygen

30% inerts

Overall Mass Balance:

SPECIES	F (mol/min)	+ B (mol/min)	= P (mol/min)	y
N ₂	3.20	0.0	3.20	0.776
O_2	0.852	0.0	0.852	0.207
CH₄	0.0	0.0354	0.0354	0.009
H ₂	0.0	0.0142	0.0142	0.003
Inerts	0.0	0.0212	0.0212	0.005
TOTALS			4.1228	1.000

MINIMUM ALLOWABLE TCCS FLOW RATE:

For Methane:

0.05P = 0.0354 mol/min

P = 0.708 mol/min

 $P = (0.708 \text{ mol/min})(0.0224 \text{ m}^3/\text{mol})(60 \text{ min/hr}) =$

 $0.952 \text{ m}^3/\text{hr} = 0.560 \text{ CFM}$

For Hydrogen:

0.04P = 0.0142 mol/m

P = 0.355 mol/min

 $P = (0.355 \text{ mol/min})(0.0224 \text{ m}^3/\text{mol})(60 \text{ min/hr}) =$

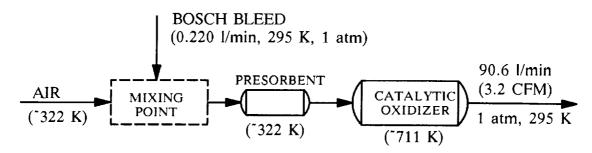
 $0.477 \text{ m}^3/\text{hr} = 0.281 \text{ CFM}$

CONCLUSIONS:

Nominal TCCS operation does not present a flammability hazard. A flammability hazard exists at worst case Bosch bleed conditions at approximately 1 m³/hr.

APPENDIX B Catalytic Oxidizer Material Balance

TCCS MATERIAL BALANCE



Bosch Bleed Composition: 0.220 l/min, 1 atm, 295 K

SPECIES	AVERAGE % VOLUME	NORMALIZED % (AVE%X[100/104.7]) VOLUME
CO ₂ H ₂ CH ₄ CO N ₂ O ₂ H ₂ O	2.2 15.6 47.1 5.3 29.0 5.0 0.5	2.10 14.90 44.99 5.06 27.70 4.78 0.48
TOTALS	104.7	100.01

Inlet Air Composition:

SPECIES	AVERAGE % VOLUME
CO ₂ O ₂ N ₂	0.093 22.32 77.58
TOTALS	99.993

Correct Air Flow Rate to 322 K

(90.6 l/min)(322 K/295 K) = 98.89 l/min

Mass Flow Rates

TCCS Inlet Air $\dot{m}_{i} = \dot{v} y_{i} M_{i} (mol/22.4 l) [1/(322 K/273 K)]$

 CO_2 : $\dot{\mathbf{m}} = (98.89 \text{ l/min})(0.00093)(44.0098 \text{ g/mol})(\text{mol}/22.4 \text{ l})$

 \times [1/(322 K/273 K)] = 0.1532 g CO₂/min

 O_2 : Similarly, $\dot{m} = 26.7 \text{ g } O_2/\text{min}$

 N_2 : $m = 81.3 g N_2/min$

Mass Flow Rates (continued)

Bosch Bleed: $\dot{m}_{1} = \dot{v} y_{1} M_{1} (\text{mol}/22.4 \text{ l}) [1/(295 \text{ K}/273 \text{ K})]$

CO₂: $\dot{m} = (0.220 \text{ l/min})(0.021)(44.0098 \text{ g/mol})(\text{mol}/22.4 \text{ l})$

 \times [1/(295 K/ 273 K)] = 0.00840 g CO₂/min

Similarly,

 H_2 : $\dot{m} = 0.00273 \text{ g H}_2/\text{min}$ CH_4 : $\dot{m} = 0.0656 \text{ g CH}_4/\text{min}$ $\dot{m} = 0.0129 \text{ g CO/min}$ $\dot{m} = 0.0705 \text{ g N}_2/\text{min}$ $\dot{m} = 0.0139 \text{ g O}_2/\text{min}$

 H_2O (v): $\dot{m} = 0.000786 \text{ g } H_2O$ (v)/min

Mass Balance at Mixing Point:

SPECIES	F (g/min)	+ B (g/min) =	P (g/min)	n (mol/min)
CO ₂	0.1532	0.00840	0.1617	0.00367
N ₂	81.3	0.0705	81.3705	2.9047
O ₂	26.7	0.0139	26.7139	0.8348
CH ₄	0	0.0656	0.0656	0.00409
H ₂	0	0.00273	0.00273	0.00135
СО	0	0.0129	0.0129	0.000460
H ₂ O (v)	0	0.000786	0.000786	0.0000436
TOTALS	108.1532	0.174816	108.328016	3.7491136

Mole Fractions after Mixing Point:

SPECIES	n (mol/min)	y _ı
CO ₂ N ₂ O ₂ CH ₄ H ₂ CO H ₂ O (v)	0.00360 2.9047 0.8348 0.00409 0.00135 0.000460 0.0000436	0.000979 0.774770 0.222666 0.001091 0.000367 0.000123 0.000012
TOTALS	3.7491136	1.000000

Material Balance at Catalytic Oxidizer: Case 1

F

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
 $CO + O_2 \rightarrow 2CO_2$
 $2H_2 + O_2 \rightarrow 2H_2O$
 $P = \sum_{i=0}^{\infty} n_{i=0UT}$

$$n_{\text{OUT}} = n_{\text{IN}} - n_{\text{REACTED}} + n_{\text{PRODUCED}}$$

Basis: 3.749 mol/min inlet, 83.1% CO, 67.3% CH_4 and, 100% H_2 oxidation From stoichiometry:

SPECIES	MOLES FED + (mol/min)	MOLES PRODUCED - (mol/min)	MOLES REACTED = (mol/min)	MOLES OUT (mol/min)
CO ₂ N ₂ O ₂ CH ₄ H ₂ CO H ₂ O (v)	0.00367 2.9047 0.8348 0.00409 0.00135 0.000460 0.0000436	0.0029856 0 0 0 0 0 0 0 0.00270	0 0 0.0060948 0.0026176 0.00135 0.000368 0	0.0066556 2.9047 0.8287058 0.0014724 0 0.000092 0.0027436
TOTALS	3.7491136	0.00569856	0.0104298	3.7443694

Outlet Composition:

	FLOW RATE	MOLE	FRACTIONS
SPECIES	n (mol/min)	у	y, Analysis Results
CO ₂ N ₂ O ₂ CH ₄ H ₂ CO H ₂ O (v)	0.0066556 2.9047 0.8287058 0.0014724 0 0.000092 0.0027436	0.00178 0.77575 0.22132 0.00039 0 0.0000245 0.00073	0.00197 0.7807 0.2223 0.00045 <0.004 0.000025
TOTALS	3.7443694	0.99999	1.005445

Material Balance at Catalytic Oxidizer: Case 2

$$\begin{array}{c|c}
\hline
F & CH_4 + 2O_2 \rightarrow CO + CO_2 + 2H_2O \\
\hline
CO + O_2 \rightarrow 2CO_2 \\
2H_2 + O_2 \rightarrow 2H_2O
\end{array}$$

$$\begin{array}{c|c}
P = \sum n_{1OUT} \\
\hline
n_{OUT} = n_{IN} - n_{REACTED} + n_{PRODUCED}$$

Basis: 3.749 mol/min inlet, 100% CO feed, 67.3% CH₄, 100% H₂ oxidation and 93% oxidation of residual CO resulting from the methane reaction

From stoichiometry:

SPECIES	MOLES FED + (mol/min)	MOLES PRODUCED – (mol/min)	MOLES REACTED = (mol/min)	MOLES OUT (mol/min)
CO ₂	0.00367	0.0029856	0	0.006656
N ₂	2.9047	0	0	2.9047
O_2	0.8348	0	0.0068602	0.8279398
CH ₄	0.00409	0	0.0026176	0.0014724
H ₂	0.00135	0	0.00135	0
CŌ	0.000460	0.000092	0.000460	0.000092
H ₂ O (v)	0.0000436	0.00270	0	0.0027436
TOTALS	3.7491136	0.00569856	0.0104298	3.7436038

Outlet Composition:

	FLOW RATE	MOLE	FRACTIONS
SPECIES	n (mol/min)	у	y, Analysis Results
CO ₂	0.006656	0.00178	0.00197
N ₂	2.9047	0.77591	0.7807
O_2	0.8279398	0.22116	0.2223
CH ₄	0.0014724	0.00039	0.00045
H ₂	0	0	< 0.004
co	0.000092	0.0000246	0.000025
H ₂ O (v)	0.0027436	0.000733	0
TOTALS	3.7436038	0.99999	1.005445

CONCLUSIONS: The material balances support the results observed for methane and carbon monoxide oxidation efficiencies of 67.3% and 83.1%. Incomplete hydrocarbon oxidation is not supported by the analysis results.

APPENDIX C Catalytic Oxidizer Energy Balance

ENERGY BALANCE Prediction of temperature rise in the catalytic oxidizer

$$Q + W = \Delta U + \Delta E_{K} + \Delta E_{P} \qquad \text{where } \Delta U = \Delta H$$

$$Q = \Delta H = \sum_{OUT} \mathbf{\mathring{n}}_{i} \hat{H}_{i} - \sum_{IN} \mathbf{\mathring{n}}_{i} \hat{H}_{I} + \sum \mathbf{\mathring{n}}_{i} \Delta \hat{H}_{IRXN}^{\circ} / \nu_{I}$$

Case 1: assume the reactor is well insulated: Q = 0

$$0 = \sum_{\text{OUT}} \stackrel{\bullet}{\mathbf{n}}_{_{\! \! |}} \hat{\mathbf{h}}_{_{\! \! |}} - \sum_{\text{IN}} \stackrel{\bullet}{\mathbf{n}}_{_{\! \! |}} \hat{\mathbf{h}}_{_{\! \! |}} + \sum \stackrel{\bullet}{\mathbf{n}}_{_{\! \! |}} \Delta \hat{\mathbf{H}}_{_{\! \! |} \, \, \mathsf{RXN}}^{\circ} / \nu_{_{\! \! |}}$$

$$T_{CAT OX} = 633 \text{ K};$$
 $T_{REF} = 298 \text{ K}$

SPECIES	HEAT CAPACITY . C _P (cal/mol)
CO ₂	10.34 + 0.00274T
N ₂	6.50 + 0.00100T
O ₂	8.27 + 0.000258T
CH ₄	5.34 + 0.0115T
H ₂	6.62 + 0.00081T
CO	6.60 + 0.00120T
H ₂ O (v)	8.22 + 0.00015T

Heat capacities, $C_p(T)$, taken to first order in T for simplification p. 3-120, Table 3-174 of the Chemical Engineers' Handbook, Fifth edition.

<u>Calculate \hat{H}_{IN} for each species</u>: $\hat{H}_{IN} = \int_{208}^{633} C_P(T) dT$

CO₂: $\hat{H}_{IN} = \int_{298}^{633} (10.34 + 0.00274T) dT = (3856 \text{ cal/mol})(4.184 \text{ J/cal}) = 16134 \text{ J/mol}$ Similarly,

 H_2 : $\dot{H}_{IN} = 9807 \text{ J/mol}$ CH_4 : $\dot{H}_{IN} = 14987 \text{ J/mol}$ CO: $\dot{H}_{IN} = 10033 \text{ J/mol}$ \dot{N}_2 : $\dot{H}_{IN} = 9761 \text{ J/mol}$ \dot{O}_2 : $\dot{H}_{IN} = 10364 \text{ J/mol}$

 H_2O : $H_{IN} = 12334 \text{ J/mol}$

Molar Flow Rates into and out of the Catalytic Oxidizer:

SPECIES	n _{IN} (mol/min)	n _{our} (mol/min)
CO ₂ N ₂ O ₂ CH ₄ H ₂ CO H ₂ O (v)	0.00367 2.90 0.835 0.00409 0.00135 0.00460 0.0000436	0.00666 2.90 0.829 0.00147 0 0.0000920 0.00274
TOTALS	3.75	3.74

$\underline{Calculate} \sum_{IN} \underline{\hat{\textbf{n}}_i} \, \hat{\textbf{H}}_i \, \text{and} \, \sum_{OUT} \underline{\hat{\textbf{n}}_i} \, \hat{\textbf{H}}_i \colon$

$$\sum_{iN} \hat{n}_i \hat{H}_i = 37143 \text{ J/min}$$

$$\sum_{OUT} \hat{n}_i \hat{H}_i = 0.01062T^2 + 108.089T - 33149$$

Solve the Energy Balance for T:

T = 703 K

$$0 = 0.01062T^{2} + 108.089T - 33149 - 37143 - 8400$$

$$T = \frac{-108.089 \pm \sqrt{(108.098)^{2} - 4(0.01062)(78692)}}{2(0.01062)}$$

The actual temperature averaged 711 K which is approximately 1% higher than predicted.

It should be noted that the analysis does not account for energy losses resulting from conduction, radiation, and other sources.

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