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SENSITIVITY OF GAS FILTER CORRELATION

INSTRUMENT TO VARIATIONS IN OPTICAL BALANCE

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> NATELAL HERMAUTICS AND SPACE ADMINISTRATION LANGUST RE HALTEN CENTER, NAMETON, VERGENIA - 1, 115

1. Report No. 2	Government Accessio	n No.	3. Recipient's Catalog	No.			
 A. Title and Subtitle Sensitivity of a Gas Filter to Variations in Optical Bal 	4. Title and Subtitle Sensitivity of a Gas Filter Correlation Instrument to Variations in Optical Balance						
7. Author(s) Harry D. Orr, III and Shirle	*	8. Performing Organization Report No. NASA TM X-17797					
9. Performing Organization Name and Address National Aeronautics and Spa Langley Research Center Hampton Virginia 23665	ation 1	642-12-12-01 1. Contract or Grant M	00 No.				
12. Sponsoring Agency Name and Address	1 1 1	3. Type of Report and ASA Technical 4. Sponsoring Agency	Memorandum Code				
15. Supplementary Notes *LTV Aerospace Corporation	Sj	pecial technical or formal NASA p	information, ublication	not planned			
[*] LTV Aerospace Corporation [*] LTV Aerospace Corporation [*] Special technical information, not planned for formal NASA publication ^{16.} Abstract The sensitivity of a simple Gas Filter Correlation Radiometer (GFCR) to variations in the instrument's optical balance parameter, τ_A , has been studied theoretically. A computer program was used to simulate the response of the GFCR to changing pollutant levels of CO, SO ₂ , CH ₄ , and NH ₃ in two model atmospheres. Positive and negative deviations of τ_A of magnitudes 0.01, 0.1, and 1 percent were imposed upon the simulation and the resulting deviations in inferred concentrations were determined. For the CO, CH ₄ , and the higher pressure cell of the NH ₃ channel, the deviations are less than [±] 12 percent for deviations in τ_A of [±] 0.1 percent, but increase to significantly higher values for larger deviations. For the lower pressure cell of NH ₃ and for SO ₂ , the deviations in inferred concentration begin to rise sharply between 0.01 and 0.1 percent deviation in τ_A , suggesting the deviation in τ_A suggesting							
17. Key Words (Suggested by Author(s)) (STAR Instrumentation and Phot Infrared Technology Instrume	category underlined) ography nt Standards	18. Distribution Statemant					
Remote Sensing Computer Atmospheric Trace Constituent	Simulation			an Price*			
19. Security Classif. (of this report) Unclassified	20. Security Classif. (Unclassifi chnical Information Serv	of this page) ed. /Ice, Springfield, Virginia 221	23. No. of Pages 47.	\$3.75			

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*Available from STIF/NASA Scientific and Technical Information Facility, P.O. Box 33, College Park, MD 20740

SENSITIVITY OF A GAS FILTER CORRELATION INSTRUMENT TO VARIATIONS IN OPTICAL BALANCE

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Harry D. Orr, III and Shirley A. Campbell

ABSTRACT

The sensitivity of a simple Gas Filter Correlation Radiometer (GFCR) to variations in the instrument's optical balance parameter, T_A , has been studied theoretically.

A computer program was used to simulate the response of the GFCR to changing pollutant levels of CO, SO₂, CH_4 , and NH_3 in two model atmospheres. Positive and negative deviations of τ_A of magnitudes 0.01, 0.1, and 1 percent were imposed upon the simulation and the resulting deviation in inferred pollutant concentration were determined.

For the CO and CH₄ channels, and the higher pressure cell of the NH₃ channel, the deviations are less than ± 12 percent for the deviations in τ_A of ± 0.1 percent, but increase to significantly higher values for larger deviations. For the lower pressure cell of the NH₃ channel and for the SO₂ channel, the deviations in inferred concentration begin to rise sharply between 0.01 and 0.1 percent deviation in τ_A , suggesting that a tighter control on τ_A may be required for this channel.

I. INTRODUCTION

The concept of measuring the total burden or column density of trace gases by nondispersive infrared techniques is currently an area of much interest. One variety of this technique, the gas filter correlation radiometer (GFCR), is being explored for both aircraft and satellite applications to the measurement of pollutant gas concentrations (refs. 1-2). The operation of the instrument depends not only upon the various parameters describing the underlying surface and atmosphere, but also upon those describing the instrument's physical state -- for example, the temperature, emissivities and reflectivities of various optical components. Moreover, the reliability of the data from such an instrument is strongly affected by the stability of these parameters. This report presents the results of a theoretical study of the sensitivity of the GFCR to one such parameter, the vacuum - cell aperture transmission, τ_A , which is used to mechanically balance the optical paths of the instrument under conditions of no pollutant gas. The role of this aperture is described in the following section. A list of symbols is given in Appendix B.

II. THEORY OF OPERATION OF GFCR

Detailed descriptions of instruments based on the gas filter correlation technique have been presented elsewhere (see, for example, refs. 1-2). In this work, only the basic elements of a prototype instrument will be described. Figure 1 is a schematic diagram of a simple GFCR. Radiation from the earth's surface and intervening atmosphere enter through the front window. One half of the energy is blocked by a chopper blade; the other half is passed through a lens, then through a cell containing a sample of the gas of interest, and is focused onto a detector. One half cycle later, the chopper blocks the energy on the right hand side and passes it on the left hand side, which contains an empty cell and an adjustable aperture. The difference between the two signals can be expressed as a differential radiance, ΔN , proportional to an instrument voltage, ΔV :

$$\Delta V \alpha \Delta N \alpha \int_{\Delta v} E(v) [C(v) \tau_{G} - C'(v) \tau_{A}] dv \qquad (1)$$

where E(v) is the incident radiation at wavenumber v, C(v), and C'(v) are the transfer functions of the optical components of the right and left hand paths, respectively, $\tau_{G}(v)$ is the wavenumber-dependent transmittance of the reference gas, and τ_{A} is the wavenumber-independent transmittance of the aperture of the vacuum cell. The filter accepts radiation in the bandpass Δv_{o} . The signals also may be combined to give an integral radiometer measurement:

$$\mathbf{V} \propto \mathbf{N} \propto \int_{\Delta \mathbf{v}} \mathbf{E}(\mathbf{v}) \left[\mathbf{C}(\mathbf{v}) \ \mathbf{\tau}_{\mathbf{G}}(\mathbf{v}) + \mathbf{C}'(\mathbf{v}) \ \mathbf{\tau}_{\mathbf{A}} \right] \, \mathrm{d}\mathbf{v} \tag{2}$$

When none of the gas of interest is present outside the instrument, the dependence of E on ν is very weakly correlated with the dependence of $\tau_{\rm G}$ on ν . In practice this condition is achieved by alternately placing a hot and then a cold blackbody at the entrance window. The change in ΔV is then minimized by mechanically adjusting the aperture transmission, $\tau_{\rm A}$. This procedure is commonly referred to as "balancing" the instrument. When the gas of interest is present outside the instrument, in the atmosphere or in a calibration cell, the dependence of E on ν is altered by absorption and emission at the same wavenumbers as are active in the instrument gas cell. This correlation produces an imbalance in the signal strengths between the two optical paths and causes the output signal to deviate from its "balance" value. At the same time, the integral radiance signal, V, is strongly related to the brightness temperature of the background surface.

III. DATA REDUCTION PROCEDURE

Since it is not currently possible to simulate accurately the infrared activity of the earth's atmosphere in the laboratory, theoretical techniques must be used to relate the voltage output of the instrument to the gas burden measured. The primary tool used in this effort is a line-by-line radiative transfer program "POLAYER" (ref. 3). For the purpose of this program, the background surface (either the earth or a laboratory source) is described by a temperature and emissivity; the intervening atmosphere is specified in the form of one or more layers with a thickness, pressure, temperature, and concentration of gases. The instrument is described in terms of the temperature and spectral transmittances of the various components of each of its optical paths. Then, the radiation reaching the detector along each of the optical paths is computed by integrating over Δv the surface radiation, as modified by any absorbing spectral lines in each layer, plus contributions by any emitting spectral lines in each layer. This procedure is employed in three stages. First, the theoretical value of τ_A is computed which will produce equal values of AN for the known laboratory sources with no gases between the sources and the instrument. Next, using this value of τ_A , a description corresponding to the calibration cell used with the instrument is inserted into the program. The results of this calculation establish a relation between the voltages measured by the instrument and the corresponding values of

radiance. The real atmosphere with its inherent non-homogeneity, cannot be simulated by such cells; thus in the third stage a description of the real atmosphere, to whatever accuracy it is known at the time of measurement, is inserted. The response of the instrument to the radiances associated with a range of potential concentrations of the gas of interest is computed. Figures 2 - 5 show the responses of the instrument to the standard atmosphere used in this study. To infer the actual concentration, the voltage calibration from stage two is used to convert the instrument output to radiance units (e.g., watts/cm² sr); then the corresponding gas concentration is found by interpolation on the response curve generated in stage three.

IV. METHODOLOGY

In the present work, the sensitivity of the GFCR was studied in four spectral regions, corresponding to wavelengths that might be used in measurement of carbon monoxide (CO), methane (CH₄), sulfur dioxide (SO₂), and ammonia (NH₃), for two pressures of the instrument gas cell (one in the case of SO₂). The details of these conditions are given in table 1.

To use the POLAYER program, two atmospheric models were constructed. In each model, the region from the surface to 22 km was divided into five layers. The layers were chosen so that each contains an approximately equal column density of gas (molecules). The details of the layers are given in table 2.

Model 1 is based on the U.S. Standard Atmosphere, 1962 (ref. 4). The mean temperature of each of the five layers was determined by weighting the U.S. Standard temperatures with the corresponding density values. The vertical distribution of water vapor was taken as that of the Gutnick Model (ref. 5).

Model 2 is based on the U.S. Standard Atmosphere Supplements, 1966, 45° N. latitude for July (ref. 6). The water vapor distribution was taken from the midlatitude summer atmospheric profile of AFCRL Optical Properties of the Atmosphere (ref. 7).

For both models, a surface emissivity of .98 was used; a nighturime measurement was assumed, hence no solar contribution was included. For Model 1, a ground temperature of 288K was used. While the concentrations of all other species

were held constant, the concentration of the pollutant gas of interest, uniformly distributed, was varied in ten steps below and above its nominal or background level. For Model 2, a ground temperature of 296K was used. The details of the distributions are given in table 2.

For each instrument channel and atmospheric model combination, seven response function curves were computed, one corresponding to the standard or correct value of τ_A and six other curves corresponding to variations in τ_A of $\pm 1\%$, $\pm .1\%$, and $\pm .01\%$ from its standard value.

To simulate measurements, four values of ΔN 'were then selected, and the corresponding values of pollutant concentration were determined by interpolation on each of the seven curves. For each of the four ΔN values, the differences between the indicated concentration in the standard case and the concentrations found in the six varied cases were calculated.

V. RESULTS

The results of the procedure described above are plotted in figures 6 - 13 and tabulated in Appendix A. Each figure, corresponding to a particular species, cell condition, and atmospheric model, shows the percent deviation of the inferred concentration as a function of the percent deviation of τ_A from its standard value.

For all cases, the relative behaviors of the deviations are similar. As τ_A is decreased from its standard values, the percent deviations in inferred concentration become increasingly negative; as τ_A is increased, the deviations become positive. The rate of change of the deviation also appears to increase with deviations in τ_A . For CO, CH₄, and cell 1 of the NH₃ channel magnitudes of deviations of inferred concentrations undergo a sharp rise as the deviations in τ_A exceed $\pm 0.1\%$. For cell 2 of NH₃ and SO₂ the rise commences at even lower deviations in τ_A .

The deviations for CO, CH_4 , and NH_3 for a given atmospheric model are lower for the cell with the higher concentration. The reason for this behavior can be seen in figures 2, 4, and 5. The response function for the cell with the higher concentration has less of a tendency to saturate in the range of

atmospheric concentrations considered. Therefore, the inferred concentration at any signal level is less sensitive to the small changes in the response function induced by variations in τ_A .

For a given species and cell concentration, the deviations in inferred concentration are of smaller magnitude for the Model 2 atmosphere than for the Model 1 standard. Although not illustrated in the figures, the reason for this situation is similar. The Model 2 atmosphere, with higher surface and atmospheric temperatures than Model 1, produces generally higher signal levels and leads to response functions with less of a tendency to saturate than those arising from Model 1. These "stiffer" response functions lead to lower deviations in inferred concentration with changes in τ_A .

VI. CONCLUSIONS

From the preceding discussion, it is clear that the sensitivity of the GFCR to variations in the balancing aperture is not a simple relationship. Not only do the deviations depend in a very nonlinear way on the magnitude of the deviation in τ_A , but also upon the particular spectral region or species considered, the concentration in the sample cell of the instrument, and the details of the surface and atmosphere over which the instrument is operated. In addition, for a given deviation in τ_A , there does not seem to be a consistent relationship between the level of inferred concentration and the deviation to be expected. In other words, for a particular τ_A , it is not possible to predict whether the greatest deviations in the inferred concentration will occur at high, intermediate, or low pollutant levels.

The complex dependence of the deviations notwithstanding, some general conclusions concerning optical balance from an operational point of view can be reached.

For the CO, CH_4 , and the higher pressure cell of the NH_3 channel, the deviations in inferred concentration will be kept within reasonable limits, i.e., to 12 percent, if τ_A is maintained to within ± 0.1 percent of its nominal value. In view of the consistently high deviation observed for the lower pressure cell of the NH_3 channel, consideration of a higher partial pressure in this cell seems warranted. It should be noted that the above

conclusions apply to the ranges of pollutant concentrations considered in this study and may not be valid for ranges significantly different from them. Also, it is evident that atmospheric and surface conditions which tend to reduce the signal levels; e.g., lower surface temperatures, and more nearly isothermal temperature profiles, will tend to increase the deviation expected at any given deviation in τ_A . For the lower pressure cell of the NH₃ channel and for the SO₂ channel, unacceptably large deviations are much more likely to occur with ± 0.1 percent tolerance on τ_A . A rough estimate of the limits on the optical balance required to give the same probability of not exceeding about ± 12 percent deviation in concentration would be ± 0.03 percent. The same qualifications, of course, apply as did to the other species; in fact, the sensitivity of the required tolerance to surface and atmospheric parameters may be even stronger in the case of the lower pressure cell of NH₃ and of SO₂ than for the other species considered.

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Table 1

				1
Species	CO	so ₂	NH3	CH ₁₄
Center Wavelength (micrometers)	4.66	8.55	11.2	8.0
Bandwidth (micrometers)	4.50 - 4.32	8.11 - 8.99	10.43 - 11.97	7.53 - 8.47
Cell Pressure (N/m ²)	1.013 × 10 ⁵	1.013 × 10 ⁵	1.013 × 10 ⁵	1.013 × 10'
Cell Length (cm)	l	1	1	l
Partial Pressure (N/m ²)				_
Cell 1	3.546 x 10 ⁴	1.013 x 10 ⁵	2.026 x 10 ⁴	1.013×10^{2}
Cell 2	1.013×10^{4}		1.013 x 10 ³	2.026 x 10 ⁴
Cell Temperature (K)	300	300	300	300
Balance Temperature (K)				
Cold	266	266	266	266
Hot	310	310	310	310
Standard Aperture Transmission (τ_A)				
Cell l	.830128	.514679	.849515	.754904
Cell 2	.915968		.982169	.904845

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INSTRUMENT PARAMETERS

					I.RActive Constituent Concentrations (ppm)						
Model	Layer	Extent (km)	Pressure (N/m ²)	Temperature (K)	^{CO} 2	н ₂ 0	N20	со	⁵⁰ 2	Сн	NH3
1	1	0 - 2	9.142 × 10 ⁴	282.02	330.	6254.	.28	.1	.005	1.	.01
	2	2 - 4	7.136	269.11	330 .	3408.	.28	.1	.005	1:	.01
	3	4 - 7	5.169	253.3 ¹	330.	1335.	.28	.1	.005	1.	.01
ľ	4	7 - 11	3.176	231.26	330.	274.	.28	.1	.005	1.	.01
	5	11 - 22	9.555 × 10 ³	216.97	330.	15.	.28	.1	.005	1.	.01
						<u> </u>					
2	l	0 - 2	9.048 × 10 ⁴	291.30	330.	14310.	.28	•5	.06	1.	.01
	2	2 - 4	7.126	280.00	330.	6529.	.28	.2	.005	1.	.01
	3	4 - 7	5.224	264.80	330.	2143.	.28	.1	.005	1.	.01
	4	7 - 11	3.279	242.80	330.	504.3	.28	.1	.005	1.	.01
	5	11 - 22	1.164	218.60	330.	17.84	.28	.1	.005	1.	.01

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DETAILS OF ATMOSPHERIC MODELS

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APPENDIX A

		Cell Partial Pressure	Cell Partial Standard $\Delta \tau_A$ Percent						
Model Speci	Species	(N/m^2)	Concentration (ppm)	-1	1	01	+.01	+.1	+1
1	со	3.546 x 10 ⁴	.05	-80.0	-8.0	-1.0	3.0	10.0	50.0
			.1	-70.0	-6.0	5	5.0	6.0	42.0
			.2	-66.0	-5.0	-1.3	1.0	6.0	40.0
			.3	-66.7	- 5 _° 3	7	•7	6.7	38.7
		1.013 x 10 ⁴	.05	-152.0	-12.0	-2.0	2.0	7.0	70.0
			.1	-140.0	-10.0	-2.0	•5	4.0	60.0
			.2	-177.0	-10.3	5	1.0	7.0	56.0
			.3	-217.0	- 9.3	3	2.0	9.7	57.0
	`50 ₂	1.013 x 10 ⁵	.005	*	-70.0	- 8.0	4.0	68.0	*
			.0075	*	-44.0	- 5.3	2.7	42.7	*
			.01	*	-28.0	- 2.0	4.0	35.0	*
			.015	*	-25.3	- 2.7	2.0	26.7	*
	Сн _ц	1.013 x 10 ⁵	•5	- 28.0	- 5.0	- 2.0	2.0	4.0	18.0 ⁻
			1.0	- 27.0	- 3.0	- 1.0	1.0	3.0	20.0
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Deviations in inferred concentration as function of atmospheric model, species, cell partial pressure, and pollutant concentration, and deviations in τ_A

		Cell Partial Pressure	Standard Pollutant	$\Delta \tau_A$ Percent						
Model	Species	(N/m^2)	Concentration (ppm)	-1	1	01	+.01	nt 01 +.1 7 3.3 5 2.0 0 4.0 0 4.0 4.0 4.0 0 4.0 3 6.7 0 8.0 1.0 6.0 0 8.0 1.0 6.0 0 5.0 $.0$ 5.0 $.0$ 5.0 $.0$ 5.0 $.0$ 38.0 $.0$ 26.0	+1	
1	Сн	1.013 x 10 ⁵	1.5	- 26.7	- 2.7	7	•7	3.3	20.0	
(001017	(cont'd)		2.0	- 32.0	- 2.0	5	• 5.	2.0	20.5	
		2.026 x 10 ⁴	•5	- 76.0	- 8.0	-4.0	2.0	4.0	42.0	
			1.0	-102.0	- 7.0	-2.0	1.0	4.0	41.0	
			1.5	-133.0	- 7.3	7	1.3	6.7	44.0	
			2.0	-110.0	- 5.0	- 1.0	1.0	8.0_	48.0	
	^{NH} 3	2.026 x 10 ⁴	.005	- 88.0	- 8.0	- 2.0	2.0	6.0	78.0	
			.01	- 52.0	- 4.0	- 1.0	1.0	5.0	45.0	
			.02	- 31.5	- 2.5	5	•5	3.5	28.0	
			.025	- 28.4	- 2.8	4	.4	2.4	24.4	
		1.013×10^3	.005	*	-40.0	- 4.0	2.0	38.0	*	
		:	.01	*	-24.0	- 2.0	3.0	26.0	*	
			.02	*	-14.5	- 1.5	2.0	19.5	*	
	- ·		.025	*	-13.2	8	1.6	17.6	*	

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APPENDIX A (Cont.)

		Cell Partial Pressure	Standard	$\Delta \tau_A$ Percent					
Model	Species	(N/m^2)	Pollutant Concentration (ppm)	-1	1	01	+.01	+.1	+1
2	со	3.546 x 10 ⁴	.05	-40.0	-4.0	-2.0	2.0	4.0	28.0
	- -		.1	-33.0	-3.0	-1.0	2.0	4.0	24.0
			.2	-32.0	-2.0	5	1.0	3.0	24.5
			.3	-31.7	-2.0	7	1.3	3.0	18.0
	со	1.013 x 10 ⁴	.05	-68.0	-4.0	-2.0	2.0	12.0	44.0
		`	.1	-64.0	-7.0	-2.0	1.0	3.0	38.0
			.2	-70.0	-8.0	-1.0	.5	1.0	36.0
			•3	-90.0	-3.3	.3	1.7	7.0	40.0
	[.] 50,	1.013 x 10 ⁵	.005	-292.0	-30.0	- 4.0	2.0	24.0	*
			.0075	-194.7	-18.7	- 2.7	1.3	17.3	; * *
			.01	-148.0	-15.0	- 2.0	1.0	13.0	*
	·		.015	-100.7	-10.7	- 1.3	.7	8.7	*
	Сн,	1.013 x 10 ⁵	.5	- 18.0	- 4.0	- 2.0	2.0	4.0	12.0
			1.0	- 18.0	- 3.0	- 1.0	1.0	2.0	12.0
			1.5	- 16.0	- 2.0	7	.7	2.7	13.3
•	•		•	•					

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		Cell Partial Pressure	Standard	$\Delta \tau_A^{Percent}$					
Model	Species	(N/m^2)	Concentration (ppm)	-1	1	01	+.01	+.1	+1
2	СНЪ	1.013 x 10 ⁵	2.0	- 15.5	- 1.5	5	.5	2.5	15.5
(Cont.)	(Cont.)	2.026×10^4	.5	- 44.0	- 6.0	- 2.0	2.0	4.0	30.0
			1.0	- 53.0	- 4.0	- 1.0 _{.0}	1.0	4.0	28.0
			1.5	- 62.7	- 4.7	- 1.3	1.3	4.7	31.3
	:		2.0	- 78.5	- 2.5	- 1.0	1.3_	5_5	34.0
	NH ₃	2.026×10^4	.005	- 34.0	- 6.0	- 2.0	2.0	4.0	32.0
			.01	- 21.0	- 3.0	- 1.0	1.0	2.0	19.0
			.02	- 13.0	- 1.5	- •5	•5	1.0	12.0
			.025	- 11.6	- 1.2	4	<u>_</u> 4	.8	10.8
		1.013×10^3	.005	*	-18.0	- 2.0	2.0	14.0	*
	4		.01	*	- 9.0	- 1.0	2.0	10.0	*
			.02	~ *	- 6.5	- 1.0	1.0	5.5	*
	,		.025	*	- 5.6	4	• .4	6.0	*

APPENDIX A (Concl.)

*For these values of the parameters, the response functions of the instrument remained below the radiance levels used to infer concentrations.

APPENDIX B

SYMBOLS

C(v)transfer function of the total optical path through the gas cell at wavenumber v C'(v) transfer function of the total optical path through the vacuum cell at wavenumber vE(v)radiance incident on the instrument at wavenumber ν $(watts/cm^2 \cdot sr cm^{-1})$ average of radiances passing through the vacuum cell and gas Ν cell, integrated over wavenumber (watts/cm² sr) ΔN difference between radiances passing through vacuum cell and gas cell integrated over wavenumber (watts/cm² sr) V instrument output signal corresponding to N (volts) instrument output signal corresponding to ΔN (volts) ΔV transmissivity of the vacuum cell aperture, optical balance τ parameter (see fig. 1) τ_G(ν) transmittance of the gas cell at wavenumber vν wavenumber $(cm^{-\perp})$ bandpass of the filter (cm⁻¹) (see fig. 1) Δν



Figure 1. - Schematic of typical Gas Filter Correlation Radiometer.









1962, for indicated partial pressure of SO₂ in instrument gas cell.







PERCENT DEVIATION IN TA



PERCENT DEVIATION IN TA



PERCENT DEVIATION IN TA





PERCENT DEVIATION IN π_A





PERCENT DEVIATION IN $\tau_{\rm A}$



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- PFRCENT DEVIATION IN TA



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PERCENT DE LA COMPANY