As of 10 June 2016

This GOES-R Level 2+ space weather Algorithm Theoretical Basis Document (ATBD) is preliminary and subject to change as the GOES-R Program prepares for a launch in late 2016.

The NOAA National Centers for Environmental Information (NCEI) is currently developing a demonstration version of the Satellite Product Analysis and Distribution Enterprise System (SPADES) which will host the L2+ algorithms. The operational SPADES will be instantiated by the National Weather Service in FY2017 to serve the needs of the Space Weather Prediction Center (SWPC).

Updated versions of the L2+ ATBDs will periodically be made available and posted to the SPADES website.

Bill Denig
NCEI

http://www.ngdc.noaa.gov/stp/space-weather/online-publications/stp_sii/spades/

NOAA NESDIS CENTER for SATELLITE APPLICATIONS and RESEARCH

GOES-R XRS.05 ALGORITHM THEORETICAL BASIS DOCUMENT
Version 1.4

Hardcopy Uncontrolled

TITLE: XRS.05 ALGORITHM THEORETICAL BASIS DOCUMENT VERSION 1.4

AUTHORS:
S. Dave Bouwer
Dr. Donald Woodraska
Dr. Tom Woods
Dr. Frank Eparvier
Dr. Kent Tobiska

APPROVAL SIGNATURES:

_____<Actual Signature Date>
<Name of Technical Approver> Date
Technical Approver

_____<Actual Signature Date>
<Name of Agency Approver> Date
Agency

XRS.05 ALGORITHM THEORETICAL BASIS DOCUMENT VERSION HISTORY SUMMARY

Version	Description	Revised Sections	Date
1.0	First Rough Draft	All	6 Nov 2010
1.1	First Distributed Draft	All	15 Jan 2010
1.2	Corrected draft (minor changes), Dave Bouwer, SET	3.0, 3.2, 3.3, 4.1, 4.2, 5.3, 5.5	7 May 2010
1.3	Corrected error equation 2	4.1	18 May 2010
1.4	Corrected version number in header and 3.4.3 output	Header (all pages)	9 Jun 2010

LIST OF FIGURES 9
LIST OF TABLES 10
LIST OF ACRONYMS 11
ABSTRACT 12
1.0 INTRODUCTION 13
1.1 Purpose of This Document 13
1.2 Who Should Use This Document 13
1.3 Inside Each Section 13
1.4 Related Documents 14
1.5 Revision History 14
2.0 OBSERVING SYSTEM OVERVIEW 14
2.1 Product Generated 17
2.2 Instrument Characteristics 17
3.0 ALGORITHM DESCRIPTION 19
3.1 Algorithm Overview 19
3.2 Processing Outline 20
3.3 Algorithm Input 21
3.3.1 Primary Sensor Data 22
3.3.2 Ancillary Data 22
3.4 Theoretical Description 22
3.4.1 Physics of the Problem 22
3.4.2 Mathematical Description 23
3.4.3 Algorithm Output 23
4.0 TEST DATA SETS AND OUTPUTS 24
4.1 Simulated/Proxy Input Data Sets 24
4.2 Output from Simulated/Proxy Inputs Data Sets 24
4.2.1 Precisions and Accuracy Estimates 24
4.2.2 Error Budget 25
5.0 PRACTICAL CONSIDERATIONS 25
5.1 Numerical Computation Considerations 25
5.2 Programming and Procedural Considerations 25
5.3 Quality Assessment and Diagnostics 25
5.4 Exception Handling 26
5.5 Algorithm Validation 26

6.0 ASSUMPTIONS AND LIMITATIONS 26
6.1 Performance 27
6.2 Assumed Sensor Performance 27
6.3 Pre-Planned Product Improvements 27
7.0 REFERENCES 27

LIST OF FIGURES

Figure 2.1. Example of the XRS-B and A channels, and the XRS B/A Ratio. 16
Figure 2.2. Example of XRS-A and B channels, and the flare temperature. 16
Figure 2.3. XRS solar diodes configuration. 18
Figure 3.1. XRS.05 Algorithm Flowchart. 21

LIST OF TABLES

Table 1.1. XRS.05 product data. 17
Table 4.1. Error budget estimates. 25

LIST OF ACRONYMS

ATBD	Algorithm Theoretical Basis Document
AWG	Algorithm Working Group
CIRES	Cooperative Institute for Research in Environmental Sciences
LASP	Laboratory for Atmospheric and Space Physics
SET	Space Environment Technologies
STAR	Center for Satellite Applications and Research
SWPC	Space Weather Prediction Center
XRS	X-ray Sensor

ABSTRACT

This document describes the XRS.05 algorithm that calculates the GOES-R XRS A/B channels ratio using the 3-second X-ray measurements. The logical flow of the algorithm is outlined, including error handling methods, how validation using proxy data sets will be accomplished, and explanations of assumptions.

1.0 INTRODUCTION

1.1 Purpose of This Document

The purpose of this document is to provide product developers, reviewers, and users with a theoretical description (scientific, algorithmic, and mathematical) of the GOES-R XRS ratio algorithm. This document will describe the design and development of the XRS.05 algorithm, which will create a ratio of the A-channel (also called short x-ray flux) over the B-channel (also called long x-ray flux) at a presumed 3-second cadence. This document provides the operational requirements for this product and defines how these requirements are met with this algorithm. The algorithm inputs, processing, and outputs are described in enough detail to design, develop, test, and implement the necessary processing software.

1.2 Who Should Use This Document

The members of the Space Weather Forecast Office and the Research and Customer Requirements Section of the SWPC should use this ATBD to verify that their operational requirements are being met by the proposed algorithm. They should also use it to understand the strengths and weaknesses of the algorithm as well as its accuracy and applicability. The STAR AIT group should use this document to integrate the algorithm into their collaborative framework environment. It should also be used by the ground segment contractor to design, develop, test, validate and implement the algorithm into the final operational processing system.

1.3 Inside Each Section

Section 2.0 OBSERVING SYSTEM OVERVIEW:
Describes the GOES-R XRS instrument and the measurements that serve as input to the algorithm.

Section 3.0 ALGORITHM DESCRIPTION:
Describes the development, theory, and mathematics of the XRS.05 algorithm. Describes the logical flow of the algorithm, including input and output flow.

Section 4.0 TEST DATA SETS AND OUTPUTS:

Describes the test data sets used to characterize the performance of the algorithm and the data product quality. Describes the results from the algorithm processing on simulated input data.

Section 5.0 PRACTICAL CONSIDERATIONS:
Discusses issues involving numerical computation, programming and procedures, quality assessment, diagnostics, and exception handling.

Section 6.0 ASSUMPTIONS AND LIMITATIONS:
Describes assumptions made in the implementation of the calculation of the XRS_A / XRS_B ratio, and assumptions made in validation, testing, and error handling of the algorithm.

Section 7.0 REFERENCES:
Relevant publications.

1.4 Related Documents

"GOES-R Series Acronym & Glossary Document", DOC/NOAA/NASA (GOES-R Program/Code 417), P417-R-LIST-0142, July 9, 2008.

GOES-R XRS.05 Ratio Test Plan and Results, Version 1.1, 2010.

1.5 Revision History

Version 1.0 November 6, 2009. S. Dave Bouwer, First draft.
Version 1.1 January 15, 2010. S. Dave Bouwer, First distributed draft
Version 1.2 May 7, 2010, S. Dave Bouwer, Revised
Version 1.3 May 18, 2010, S. Dave Bouwer, minor corrections
Version 1.4 June 9, 2010, S. Dave Bouwer, minor corrections

2.0 OBSERVING SYSTEM OVERVIEW

The GOES XRS measurements have been a crucial component of space weather operations since 1975, providing an accurate measurement of geo-effective X-ray irradiance from second-to-second real-time conditions to solar-cycle time scales. The integrated 0.1–0.8 nm irradiance is the definitive metric for solar flare classifications, and is a keystone in SWPC operations. Combined with

the integrated 0.05–0.4 nm irradiance, the XRS ratio can be used to provide forecasters with advanced information on flare magnitude and temperature, thus allowing early warnings of major flares to be issued. Additionally, the XRS ratio can be used as a component in subsequent automated event detection algorithms. Figure 2.1 below illustrates this phenomena using an example of a well-defined flare on April 21, 2002. The ratio reaches a maximum about 20 minutes prior to the two X-ray channel maxima.

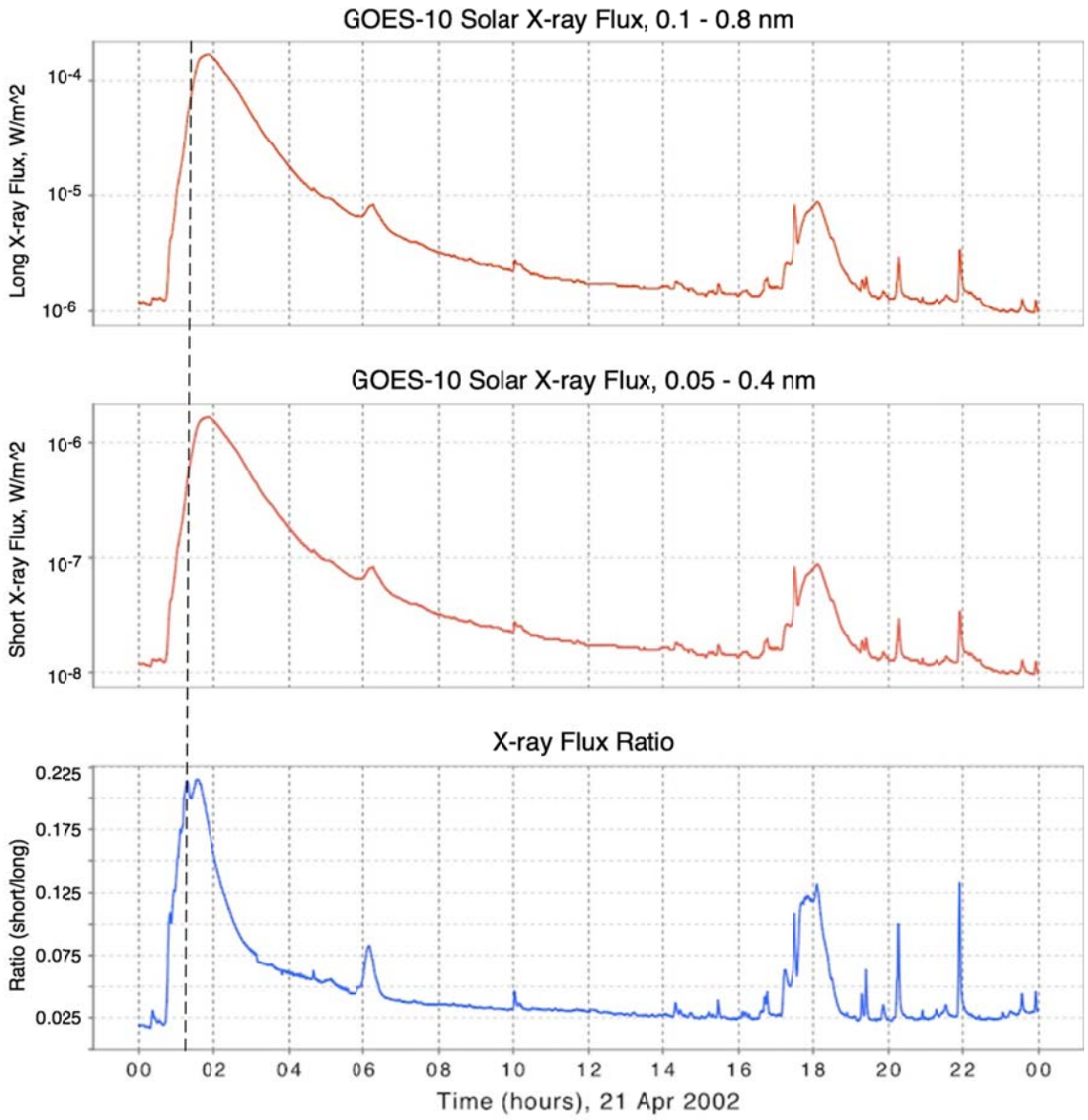

Figure 2.1. Example of the XRS-B and A channels, and the XRS B/A Ratio.

Below, Figure 2.2 illustrates the irradiance of the XRS-A and XRS-B channels during a flare on 21 Apr 2002, and the estimated flare temperature derived from the ratio. The ratio reaches a maximum before the individual XRS channels achieve their respective maxima, aiding in flare detection and prediction. Under non-flaring conditions, the ratio provides an estimate of the mean solar coronal temperatures. This information is useful not only for describing real-time solar flare evolution, but has value for subsequent scientific studies to understand the solar physics of the corona and active region evolution.

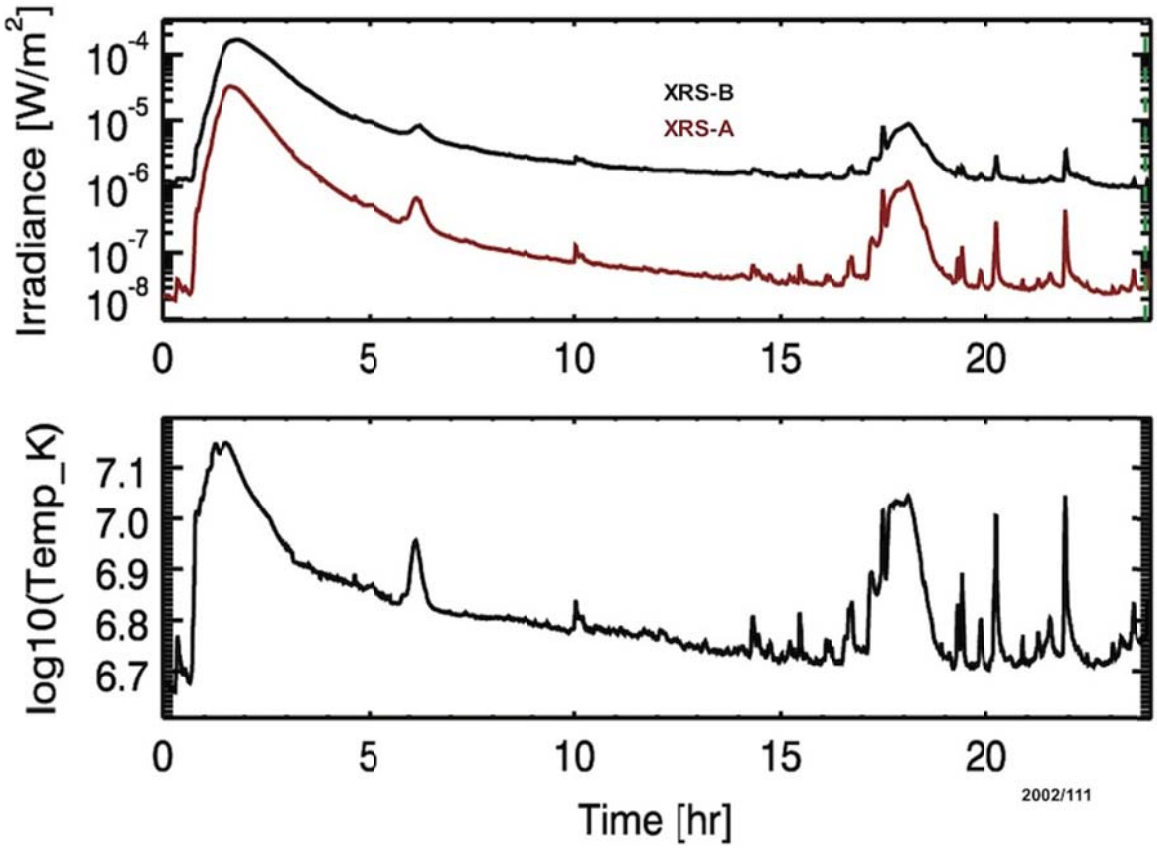

Figure 2.2. Example of XRS-A and B channels, and the flare temperature.

2.1 Product Generated

The XRS.05 ratio algorithm is the simple ratio of the "short" X-ray flux A channel (the integrated spectrum from 0.05 nm to 0.4 nm) divided by the "long" X-ray flux B channel (the integrated spectrum from 0.1 nm to 0.8 nm). However, because the measurements of X-ray flux will occur at a cadence of 0.1–3.0 seconds, and because subsequent products depend on the XRS data being verified, the algorithm needs to be designed to be extremely robust and computationally efficient. Consequently, status information on the individual channels will accompany the XRS.05 ratio calculation in real-time.

Thus the following data will be included in the XRS.05 ratio product:

Table 1.1. XRS.05 product data.

Data	Value	Note
XRS A status flag	0: missing 1: verified 2: out of range	Ratio only calculated if both A and B are verified
XRS B status flag	0: missing 1: verified 2: out of range	Ratio only calculated if both A and B are verified
XRS Ratio status flag	0: missing 1: verified	If A or B is missing or out of range, the ratio is flagged as missing
XRS Ratio	XRS-A / XRS-B	XRS.05 ratio product

2.2 Instrument Characteristics

The XRS instrument is described in detail by Chamberlin et al (2009). A brief summary is as follows:

Prior to GOES-R, the XRS instrument measured X-ray flux using two bandpass channels from a heritage design employing an ion-chamber. These channels are commonly referred to as the XRS-A (0.05-0.4 nm) and XRS-B (0.1-0.8 nm), both of which are in the soft X-ray portion of the electromagnetic spectrum. The ion-chamber design has two limitations: it 'bottom-outs' during low periods of solar activity, and is unable to effectively measure X-ray flux $\Phi < 1.0 \times 10^{-8}$ W/m^2, and the instrument saturated during major flares ($\Phi > 1.7 \times 10^{-3}$ W/m^2).

The primary goal of the re-designed XRS instrument is to continue the XRS measurements in the same spectral channels, while improving on the limitations of the legacy instrument. The new XRS instrument design addresses these limitations, while adding additional capabilities. The changes include using Si photodiodes instead of ionization cells, using multiple channels to allow wider dynamic range, providing quadrant photodiodes for real-time flare location measurements, and improved detailed calibrations using the NIST Synchrotron Ultraviolet Radiation Facility (SURF) in Gaithersburg, Maryland.

The new design will provide irradiance range of more than 6 orders of magnitude by including two photodiode sets covering different portions of the irradiance range for each of the XRS A and B channels, XRS-A1 and XRS-A2, and a similar specification for XRS-B (B1 and B2).

Figure 2.3 below illustrates the instrument solar diode sensors that measure both the XRS-A and XRS-B channels, in addition to “dark” photodiodes to measure background signal variations, and the configuration of the quadrant photodiodes for flare location determination.

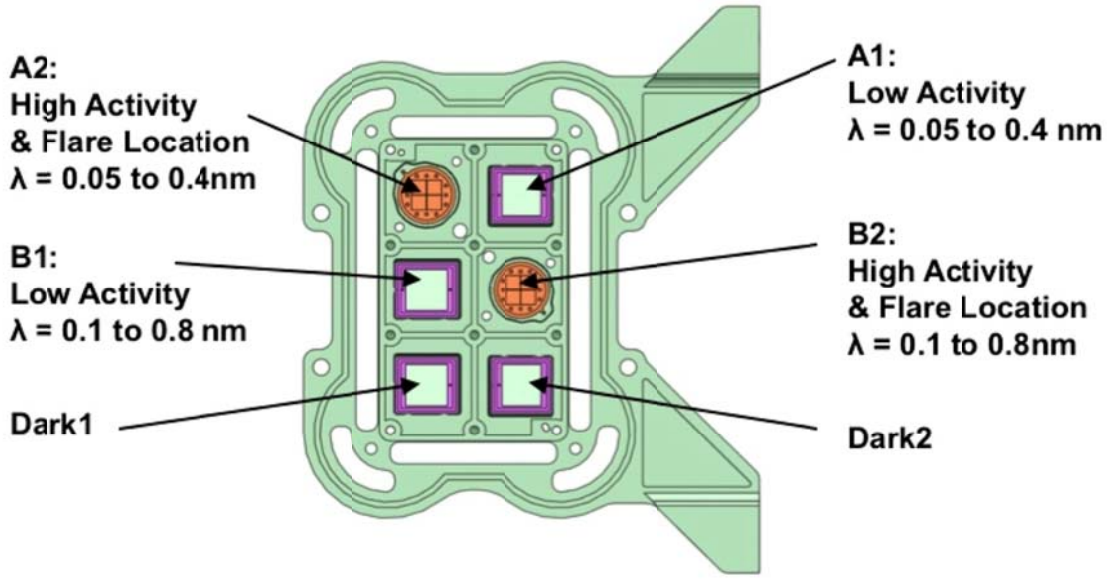

Figure 2.3. XRS solar diodes configuration.

3.0 ALGORITHM DESCRIPTION

The XRS.05 ratio algorithm will be designed to be robust (i.e., all exception conditions are anticipated and only valid data is passed on), and be computationally efficient (i.e., the algorithm must perform all operations in less than 0.1 seconds). These requirements can easily be met. The algorithm will include output quality flags for improved utility in subsequent processes and products (e.g., 1-minute averages).

The algorithm will be designed to be a callable routine for increased flexibility and extensibility in final implementation. It is expected it will be running continuously (i.e., in an “infinite loop”), and will demonstrate no “memory leaks” or other computational exceptions resulting in failure or errors. In other words, the algorithm will be designed with a “Trust, but verify” philosophy to ensure maximum fault-tolerance.

The algorithm design is language-independent, easily implemented in Fortran, C/C++, or Java. However, the XRS.05 code will be delivered in the Fortran programming language. The XRS.05 algorithm will be compatible with Level 1b software (can be run at any level).

3.1 Algorithm Overview

The algorithm will be a callable subroutine or object, so it is assumed the caller of the subroutine will provide it input of the real-time data in data tables or a similar data array structure. Correspondingly, the algorithm will return output data to the caller in a data table or array structure.

XRS Level 1b processing algorithms identify which set of channels (i.e., the low-activity A1 and B1, or the high-activity A2 and B2 channels) that should be used for generating the higher-level XRS products, so this algorithm assumes that operation is done prior to its execution. As a result, this algorithm does not have to “know” whether the input is low-activity A1/B1 or high-activity A2/B2 channels; the algorithm is independent of the channel set.

The data are assumed to be in calibrated scientific units of Watts/m^2. The algorithm will assume time values corresponding to the measurement data values are accurate. The cadence of data is expected to be 0.1-3.0 seconds.

3.2 Processing Outline

The calculation of the ratio by itself is straightforward; most of the algorithm attends to data exceptions. Figure 3.1 below presents a flowchart outlining the sequence of operations. Briefly, the sequence of operations are:

- First, examine the XRS-A and XRS-B verification flags sent in from the Level 1b to determine any pre-existing invalid status flags (i.e., preliminary verification)
- Verify XRS-A and XRS-B flux values, performing min/max comparisons (i.e., calculation verification)
- Calculate A/B ratio and the relative error of the ratio
- Assemble status information, send output back to caller

The XRS-A, XRS-B, and ratio data values will have a missing-value flag (a data value equal to -1.0×10^{-5}) substituted for a data value in the event of an exception. This is done to maintain consistency with existing GOES X-ray data products at SWPC. In addition, The XRS-A, XRS-B, and ratio status flags sent back to the caller will have one of three values:

- 0: The data value is missing
- 1: The data value is verified
- 2: The data exceeds min/max boundaries

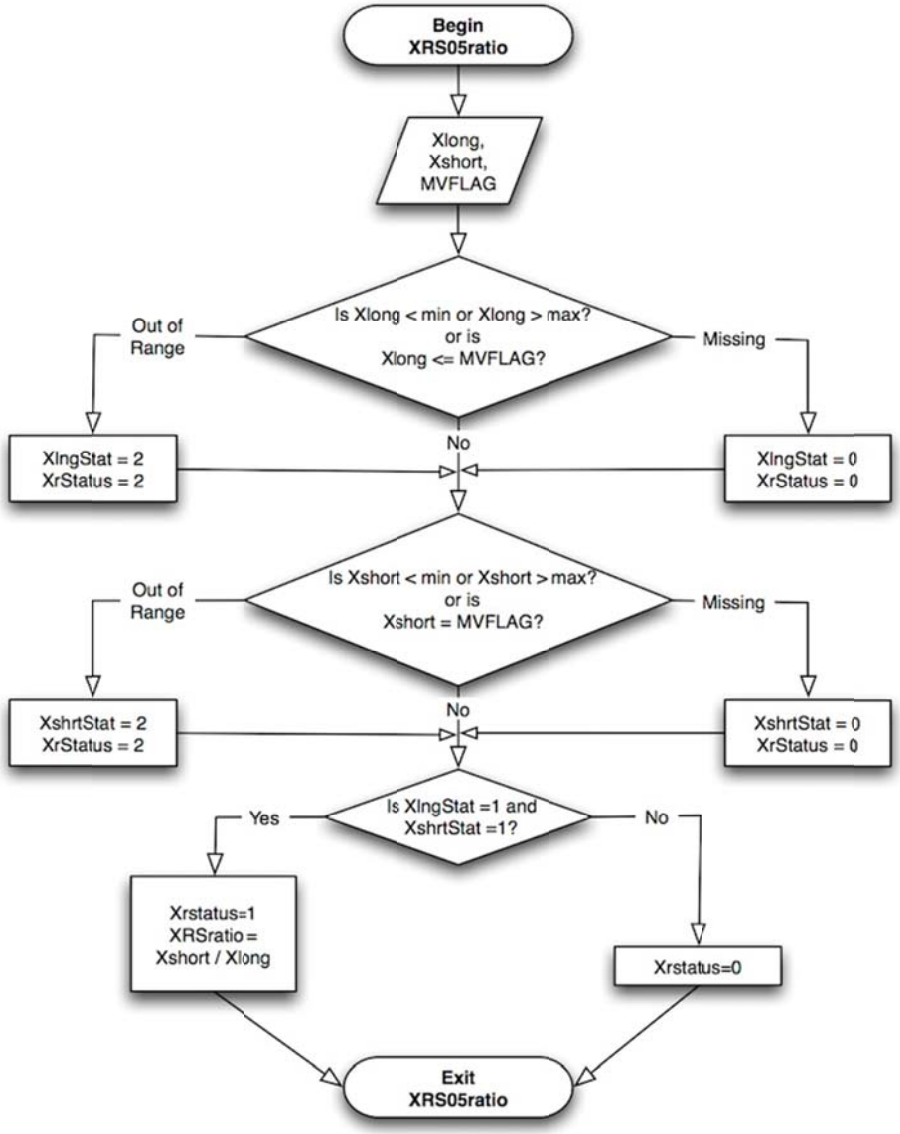

Figure 3.1. XRS.05 Algorithm Flowchart.

3.3 Algorithm Input

- Data:
  - XRS_A = Integrated spectrum from 0.05 nm to 0.4 nm, in calibrated science units

  - XRS_B = Integrated spectrum from 0.1 nm to 0.8 nm, in calibrated science units
  - Julian Day (unused in calculations, maintained as a pass-through attribute)

- Level 1b Metadata:
  - XRS_A verification flag (0 missing, 1 verified, etc.)
  - XRS_B verification flag (0 missing, 1 verified, etc.)
  - Designated missing-data flag (i.e., -1.0×10^{-5} W/m^2)
  - Valid XRS_A minimum and maximum values
  - Valid XRS_B minimum and maximum values

3.3.1 Primary Sensor Data

GOES-R XRS has six channels (Chamberlin et al., 2009): XRS-A1 & XRS-B1 are larger Si diodes to measure low X-ray flux, and XRS-A2 & XRS-B2 are smaller, quadrant Si diodes to measure high X-ray flux, and to also provide approximate flare location on the solar disk. The 'A' channels measure the integrated 0.05-4.0 nm X-ray flux, and the 'B' channels measure the integrated 0.1-0.8 nm flux. The XRS.05 ratio algorithm is independent of which set of channels are used, as other Level 1b software will select the best set to use.

3.3.2 Ancillary Data

The XRS.05 ratio algorithm is a low-level subroutine that simply calculates XRS_A / XRS_B. There are no relevant ancillary data.

3.4 Theoretical Description

The calculation of the XRS.05 XRS-A / XRS-B ratio by itself is straightforward; most of the algorithm attends to data verification. The algorithm must execute in less than 0.1 seconds. The algorithm will be a stand-alone subroutine other software can execute.

3.4.1 Physics of the Problem

The XRS-A / XRS-B ratio is generally expected to always be less than one, assuming there are no data errors. During the early rise of an X-ray flare (on the order of minutes), the XRS-A (0.05 – 0.4 nm) integrated irradiance may increase

faster compared to the XRS-B (0.1–0.8 nm) integrated irradiance as the flare evolves. Often during a flare, the XRS-A may reach a maximum value about 5 - 30 minutes sooner than the XRS-B channel (but the XRS-A value will still be lower than the XRS-B value).

Uses of this ratios information include forecasters issuing alerts and warnings and calculating the flare temperature (Woods et al., 2008). Additionally, during non-flare conditions the ratio provides the mean temperature of the solar corona (Garcia, 1994).

3.4.2 Mathematical Description

The calculation of the ratio is straightforward:

Equation 1. XRS_Ratio(t) = XRS_A(t) / XRS_B(t), t = 00, 03, 06, … (seconds)

The algorithm will first verify the Level 1b XRS_A and XRS_B inputs by testing the two channels to ensure there are no overflow/underflow exceptions that can result if the A or B channels are below a minimum value or equal to zero, above a maximum that is beyond the instruments capability, or flagged as a missing value.

From Table 1 of Chamberlin (2009), the minimum XRS-A requirement is 10^{-9} W/m^2, and the maximum XRS-B requirement is 10^{-3} W/m^2. We want max/min boundaries that are beyond the bounds of the instrument to ensure all potentially valid data are included, yet sufficiently close to the boundaries to exclude data that can clearly be classified as erroneous. The following compromise of max/min boundaries to detect out-of-range data are recommended:

- Minimum valid boundary: 1.0×10^{-11} W/m^2
- Maximum valid boundary: 1.0×10^{-1} W/m^2

3.4.3 Algorithm Output

XRS_Ratio – Unitless (A missing-value data flag equal to 0) is substituted for the ratio if an exception is detected in any of the data prior to calculation.

- XRS_A_Status_Flag,
    - 0: missing
    - 1: verified (not missing and within range)
    - 2: out of range
- XRS_B_Status_Flag,

  - 0: missing
  - 1: verified (not missing and within range)
  - 2: out of range
- Ratio_Status_Flag
  - 0: missing (either XRS_A or B are missing or out of range)
  - 1: verified

4.0 TEST DATA SETS AND OUTPUTS

Because the GOES XRS X-ray A and B channels have made measurements for over 30 years, there is a considerable amount of data at hand that can be used to test the XRS.05 algorithm.

4.1 Simulated/Proxy Input Data Sets

Three-second X-ray A and B channel data can be assembled from existing GOES XRS databases that can be used for an ensemble of test scenarios:

- Solar minimum, data missing or out of range
- Solar maximum, data near or past the upper instrument cut-off
- Moderate periods of solar activity when flares are present

A collection of data files will be assembled for each of these scenarios, and will be used to ensure the algorithm is performing correctly, based on known instances.

4.2 Output from Simulated/Proxy Inputs Data Sets

The output will be only the ratio XRS-A / XRS-B, and the three status flags:

- Ratio: XRS-A / XRS-B,
- XRS-A status flag
- XRS-B status flag
- Ratio status flag

4.2.1 Precisions and Accuracy Estimates

According to the item ID: EXISPORD81 (417-R-EXISPORD-0116, 2008), the absolute measurement accuracy of the XRS irradiance products shall be 20% (1 sigma) for each of the channels. The relative accuracy estimate shall be no more than 10%. Accounting for the two channels, the relative error for the ratio can be estimated from:

Equation 2.

$$\sigma_{A/B} = \sqrt{X_{Ratio}\left(\sigma_A^2 / X_A^2 + \sigma_B^2 / X_B^2\right)}$$

4.2.2 Error Budget

Given the estimated errors passed into the algorithm from Level 1b data, the worst case estimated errors will be (see 3.3 and 4.2.1):

Table 4.1. Error budget estimates.

Components	Standard Deviation
XRS-A	10%
XRS-B	10%
Ratio A/B	10%

5.0 PRACTICAL CONSIDERATIONS

The only potential change to the XRS.05 algorithm that may be required is if the Level 1b software redefines inputs from what are described in this document.

5.1 Numerical Computation Considerations

The lifecycle of algorithm must be no more than 0.1 sec. This is easily achieved. The data is expected to be at a 3-second cadence, but that may change after the Level-1b data is finally defined.

5.2 Programming and Procedural Considerations

The XRS.05 algorithm will be written in the Fortran computer language.

5.3 Quality Assessment and Diagnostics

The key goals for testing the algorithm are:

- Ensure the algorithm handles any potential exceptions (i.e., missing data)
- Ensure the algorithm performs all calculations within 0.1 seconds
- The algorithm, when run continuously, does not result in a “hung” condition or it does not result in any “memory leaks”

These goals can be met by developing a test-bed program that encapsulates the algorithm, reading from data files the simulated input data, then piping the data to the algorithm, and finally retrieving the simulated output data. This test-bed will provide statistics on the performance of the XRS.05 algorithm (i.e., completed

calculations per second). This test-bed program is used in lieu of a currently defined framework.

These tests will be performed on a typical Unix computer, with approximately a processor speed of 2 GHz.

5.4 Exception Handling

The algorithm shall trap all exceptions, and in the event either of the channels is flagged as missing or out of range, the ratio will be flagged as missing.

5.5 Algorithm Validation

The XRS.05 algorithm will be tested with 3 data sets from GOES-10 data archives:

- A small selection of 3-second data during solar maximum (e.g., November 2003), when X-ray flux reaches the upper saturation limit (e.g., 10^{-3} W/m^2), to test exception handling
- A small selection of 3-second data near solar minimum (e.g., June 1996), when the X-ray flux is at the lowest instrument cut-off, (e.g., 10^{-8} W/m^2), to test exception handling.
- 30 days of 3-second data during solar minimum (e.g., June 1996), to test performance

Subsequent to the ratio calculation, the ratio data will be checked to ensure the ratio behaves as expected (i.e., missing or out-or-range data are properly flagged).

6.0 ASSUMPTIONS AND LIMITATIONS

It is assumed that Level 1b data has:

- Determined which of the Low/High Activity channels to use, creating a single XRS_A and single XRS_B channel out of the four potential candidates
- Has assigned a verification flag for each of the channels. A potential limitation is that it has not trapped all exceptions, or that the flags may have additional values not relevant to the algorithm

6.1 Performance

The lifecycle of the algorithm (i.e., time to completed calculations from receipt of input to the output of data) shall be less than 0.1 seconds.

6.2 Assumed Sensor Performance

It is assumed the XRS instrument will operate within design requirements as specified in EXISPORD81 (417-R-EXISPORD-0116, 2008).

6.3 Pre-Planned Product Improvements

There are no pre-planned product improvements.

7.0 REFERENCES

Chamberlin, P. C., F. G. Eparvier, A. R. Jones, and T. N. Woods, Next Generation X-Ray Sensors (XRS) for the NOAA GOES-R Series Satellites, SPIE Proceedings, in preparation, 2009.

Garcia, H. A., Temperature and emission measure from GOES soft X-ray measurements, Solar Physics, 154, 275, 1994.

Woods, T. N., P. C. Chamberlin, W. K. Peterson, R. R. Meier, P. G. Richards, D. J. Strickland, G. Lu, L. Qian, S. C. Solomon, B. A. Iijima, A. J. Mannucci, and B. T. Tsurutani, XUV Photometer System (XPS): Improved irradiance algorithm using CHIANTI spectral models, Solar Physics, 249, doi 10.1007/s11207-008-9196-6, 2008

NASA/GOES-R/Code 417, GOES-R EUVS XRS Irradiance Sensors (EXIS), Performance and Operational Requirements Document (PORD), Document Ref: 417-R-EXISPORD-0116, Vers. 2.3, June 25, 2008.