

SpectrumImageAnalysisPy

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1 Revision History

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Contents

1	Revision History	i
2	Reference Material	iii
2.1	Table of Units	iii
2.2	Table of Symbols	iii
2.3	Abbreviations and Acronyms	iv
3	Introduction	1
3.1	Purpose of Document	1
3.2	Scope of Requirements	1
3.3	Characteristics of Intended Reader	1
3.4	Organization of Document	1
4	General System Description	2
4.1	System Context	2
4.2	User Characteristics	2
4.3	System Constraints	2
5	Specific System Description	3
5.1	Problem Description	3
5.1.1	Terminology and Definitions	3
5.1.2	Physical System Description	4
5.1.3	Goal Statements	4
5.2	Solution Characteristics Specification	4
5.2.1	Assumptions	4
5.2.2	Theoretical Models	5
5.2.3	General Definitions	6
5.2.4	Data Definitions	7
5.2.5	Instance Models	8
5.2.6	Data Constraints	12
5.2.7	Properties of a Correct Solution	12
6	Requirements	12
6.1	Functional Requirements	12
6.2	Nonfunctional Requirements	13
7	Likely Changes	14
8	Traceability Matrices and Graphs	15
9	Appendix	18
9.1	Symbolic Parameters	18

2 Reference Material

This section contains reference information to enable the reader to better understand the document.

2.1 Table of Units

Throughout this document the system of units standard to the field of electron microscopy is used as the unit system, for consistency with relevant literature and practices. For each unit, the symbol is given followed by a description of the quantity described by the symbol and the unit name.

symbol	quantity	unit name
nm	length	nanometre
eV	energy	electron volt

2.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units. The symbols are listed in alphabetical order.

symbol	unit	description
I	counts	Intensity
$b(k)$	counts	Background signal on a detector
$g(k)$	None	Gain value at each pixel
k	None	pixel index
$N(k)$	counts	Noise signal from the detector
$S(k)$	counts	Signal entering the detector
$\zeta(k)$	counts	Signal at each pixel as read out by a detector

2.3 Abbreviations and Acronyms

symbol	description
3D	Three-dimensions
A	Assumption
CCD	Charge-Coupled Device
CL	Cathodoluminescence Spectroscopy
DD	Data Definition
EELS	Electron Energy Loss
EELS	Electron Energy Loss Spectroscopy
GD	General Definition
GS	Goal Statement
IM	Instance Model
LC	Likely Change
PS	Physical System Description
PSF	Point Spread Function
R	Requirement
SI	Spectrum Image
SRS	Software Requirements Specification
STEM	Scanning Transmission Electron Microscope
SEM	Scanning Electron Microscope
SpectrumImageAnalysisPy	SpectrumImageAnalysisPy
T	Theoretical Model

3 Introduction

Three-dimensional datasets are produced by many spectro-microscopy techniques: techniques in which the response of a sample is mapped in two spatial domains and one spectral dimension. The visualization of 3D spectro-microscopy datasets is a challenging and often non-intuitive task. The motivation behind this software is to enable easy visualization and navigation through a 3D dataset to discover the features of the sample in both spatial and spectral domains. The data processing methods of 3D datasets are not trivial to perform and require a dedicated software designed to handle 3D data. This document provides the Software Requirements Specification (SRS) for a software designed to visualize and process 3D spectro-microscopy datasets derived from electron energy loss spectroscopy or cathodoluminescence.

3.1 Purpose of Document

This document details the requirements of the software `SpectrumImageAnalysisPy`. The responsibilities of the user and software are laid out and the requirements that the software must satisfy are explicitly detailed.

3.2 Scope of Requirements

The scope of the requirements for the software `SpectrumImageAnalysisPy` is limited to the import; removal of instrumentation artifacts; visualization and navigation through; and the export of EELS and CL spectrum imaging data.

3.3 Characteristics of Intended Reader

The reader of this document should have an understanding of spectrum imaging techniques, particularly EELS and the data processing methods used to remove effects of the acquisition system from the data acquired. A basic knowledge of convolution theory will be helpful to the reader and an understanding of the characteristics of 3D datasets. The reader should understand EELS and CL, as relevant to the sections of the document.

3.4 Organization of Document

The document follows the organizational scheme laid out by Smith *et al* [1, 2], starting with general reference material for the reader. The introduction of the document details the purpose of the document and intended reader, and is followed by the General System Description. The Specific System Description reduces the problem under consideration to a set of clearly defined definitions and models. The Requirements section of the document clearly outlines both the Functional and Non-functional requirements that the software must comply with. Finally, the document contains a list of Likely Changes to the software and Traceability matrices and graphs.

4 General System Description

This section identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints.

4.1 System Context

Use of the software SpectrumImageAnalysisPy infers the following responsibilities on the part of the user, and confers the following responsibilities from the program.

- User Responsibilities:
 - Provide the correct input data to the program;
 - Be capable of interacting with the software via a mouse and keyboard;
 - Have the necessary dependencies for the program installed;
 - Possess sufficient knowledge on what processing steps need to be performed and be able to judge that the quality of the output data is sufficient for the application, or change the processing steps performed;
- SpectrumImageAnalysisPy Responsibilities:
 - Read inputs (either files or data arrays) and check the inputs for the correct data type and size
 - Display the data and graphical user interface for the user to interact with
 - Respond to user commands as appropriate, including visualization and data processing commands
 - Export data in the correct file format(s)

4.2 User Characteristics

The end user of SpectrumImageAnalysisPy should be familiar with the concept of a spectrum image and an understanding of what the data represents and the appropriate actions needed to process spectrum images and extract useful information. A basic familiarity with programming is expected. An understanding of the spectro-microscopy technique (CL or EELS) used to generate the data will be beneficial, but is not strictly required.

4.3 System Constraints

The software must be able to read .dm3 files for EELS data import, and .h5 files for CL data import to be able to interface with output from the data acquisition software.

5 Specific System Description

This section first presents the problem description, which gives a high-level view of what the program is expected to do. The solution characteristics specification follows, detailing the assumptions that the software will make; the theoretical models the data analysis is based on; definitions for the types of data that the software must be able to process; and the instance models, which detail the data processing algorithms that the software will implement.

5.1 Problem Description

SpectrumImageAnalysisPy is a software to allow users to import, process, navigate, and export spectrum image data.

5.1.1 Terminology and Definitions

This subsection provides a list of terms that are used in the subsequent sections and their meaning, with the purpose of reducing ambiguity and making it easier to correctly understand the requirements:

- Cathodoluminescence: a technique in a STEM or SEM in which light emitted from the sample is collected by a mirror and directed to a spectrometer or other analysis system;
- Charge-Coupled Device: the camera used in the spectrometer to collect signal and output to the microscope acquisition software;
- Electron energy loss spectroscopy: a technique performed in a TEM or STEM which detects the energy lost by an electron beam after passing through a sample;
- Spectrum Image: a 3D dataset with two spatial dimensions and one spectral dimension, obtained using spectro-microscopy techniques (*i.e.*, EELS or CL);
- Point Spread Function (PSF): a function representing the spreading in the spectrometer, as defined in DD3;
- Spectrometer: an instrument attached to a microscope and equipped with a CCD or equivalent camera;
- Scanning electron microscope: a microscope which uses an electron beam to probe the sample and acquires data based on scattering off the surface or near the surface of the sample, operating using a raster scan of the electron beam;
- Scanning transmission electron microscope: a TEM with the capability of scanning the electron beam in a raster scan over the sample;

- Transmission electron microscope: a microscope which uses an electron beam to probe a sample and collects the signal of the transmitted beam;
- Sample: a physical sample of scientific interest that has been probed by the beam in the EELS or CL instrument.

5.1.2 Physical System Description

The physical system that the program is concerned with the analysis of includes the following elements:

PS1: Sample under study.

PS2: STEM equipped with EEL spectrometer.

PS3: SEM or STEM equipped with CL collection system.

5.1.3 Goal Statements

Given a spectrum image dataset collected by either EELS or CL and a desire to visualize and process this dataset, the goal statements for SpectrumImageAnalysisPy are:

GS1: Import a 3D dataset and display it such that the user can interact with it and navigate all three dimensions

GS2: Provide processing options including: normalization and deconvolution for EELS SI; normalization and background subtraction for a CL SI

GS3: Extract slices from the dataset as desired by the user and communicated through the user interface, export these as desired by the user

5.2 Solution Characteristics Specification

The instance models that govern SpectrumImageAnalysisPy are presented in Subsection 5.2.5. The information to understand the meaning of the instance models and their derivation is also presented, so that the instance models can be verified.

5.2.1 Assumptions

This section simplifies the original problem and helps in developing the theoretical model by filling in the missing information for the physical system. The numbers given in the square brackets refer to the theoretical model [T], general definition [GD], data definition [DD], instance model [IM], or likely change [LC], in which the respective assumption is used.

- A1: The EELS data can be described as the convolution of the “real” spectrum of the sample with the response of the microscope and spectrometer system function. The microscope and spectrometer system typically causes broadening in the peaks of the “real” spectrum;
- A2: The same PSF is valid for all pixels in the EELS spectrum image;
- A3: Fluctuations in the intensity of the EELS signal are due to changes in the beam current as collected by the spectrometer;
- A4: A subtraction is sufficient remove the contributions of the dark signal and the substrate signal from the CL sample signal;
- A5: The CL spectrometer wavelength sensitivity can be accurately modelled by experimental reference data.

5.2.2 Theoretical Models

This section focuses on the general equations and laws underlie the data acquisition process on a camera, providing the motivation for the data processing models that SpectrumImageAnalysisPy will implement.

Number	T1
Label	Intensity
Equation	$\zeta(k) = g(k)S(k) + b(k) + N(k)$
Description	<p>The signal, $\zeta(k)$ (T2), obtained from each pixel, k, on the CCD detector can be considered as a sum of several different contributions:</p> <ul style="list-style-type: none"> • the signal obtained from the microscope $S(k)$, which is multiplied by the gain factor $g(k)$ of the pixel; • the background signal of each pixel $b(k)$; • and the noise present at each pixel $N(k)$.
Source	[3]
Ref. By	DD3

Number	T2
Label	Signal
Equation	$S(k) = \int_{pixel} d\rho [\int f(\rho') h(\rho, \rho') d\rho']$ $S(k) = \sum_{k'} f(k') h(k, k')$
Description	<p>The signal ($S(k)$) from the microscope, as read at one pixel on the CCD (k), is an integral over the area of one pixel. Inside the integral is the probability ($f(\rho')$) of an electron landing at position ρ' on the detector given the interaction of the beam with the sample, multiplied by the probability ($h(\rho, \rho')$) of detecting an electron at location ρ if the electron arrives at position ρ' on the detector. The probability $h(\rho, \rho')$ of detecting an electron at one location after it hits the detector at another location is the point spread function (PSF: DD3).</p> <p>The second equation is the discretized version of the first. The signal $S(k)$ is the sum over all pixels k' of the probability ($f(k')$) of an electron hitting pixel k' multiplied by the probability ($h(k, k')$) of detecting an electron at k after it hits pixel k'.</p>
Source	[3]
Ref. By	T1 DD1 DD3

5.2.3 General Definitions

This section provides a definition beneficial to understanding the data definitions.

Number	GD1
Label	Scanning grid
Units	nm
Equation	$P(x, y) = \{\langle x, y \rangle \in A^2 \mid x \in \{0..X\}, y \in \{0..Y\}\}$
Description	<p>$P(x, y)$ is a set of position coordinates describing the possible locations of the beam in two spatial coordinates (x, y) during a raster scan across the sample in a rectangular grid pattern across the area on the sample, A^2. The limits on (x, y) are set by the operator on the instrument, ranging from 0 to the maximum (X, Y).</p>
Ref. By	DD2

5.2.4 Data Definitions

This section collects and defines the data types needed to build the instance models.

Number	DD1
Label	Spectrum
Symbol	$I(E)$
Units	Electron counts (EELS) Photon counts (CL) or arbitrary units (a.u.) for EELS or CL
Equation	$E = f(k)$ $I(E) = \zeta(k = 0..K)$
Description	Each pixel (k) on the spectrometer CCD has an energy loss (EELS) or wavelength (CL) value associated with it (E), obtained from the spectrometer acquisition settings (denoted here by $f(k)$), and a collected signal ($\zeta(k)$, T2). The intensity of the spectrum ($I(E)$) is obtained from the collected signal over the whole CCD, from the 0th pixel to the final (K th) pixel.
Sources	[4]
Ref. By	T2, DD2, DD3, IM1

Number	DD2
Label	Spectrum Image
Symbol	$I(x, y, E)$
Units	Electron counts (EELS) Photons (CL) or arbitrary units (a.u.) for EELS or CL
Equation	$I(x, y, E) : \forall \langle x, y \rangle \in P(x, y), \exists I(x, y, E) \in \mathbb{R}$
Description	$I(x, y, E)$ is a dataset composed of Spectra (DD1) collected by the spectrometer detector at each value of $P(x, y)$ (GD1).
Sources	[5]
Ref. By	DD3, IM1

Number	DD3
Label	Point Spread Function
Symbol	$I_{PSF}(E)$
Units	Electron counts or arbitrary units (a.u.) (EELS)
Equation	$I(E) = \zeta(k = 0..K) = g(k)S'(k) + b(k) + N(k)$
Description	$I_{PSF}(E)$ is a reference spectrum ($I(E)$, DD1) representing the effect of the point spread function (see T2) on the collected spectra in the spectrum image (DD2). It is a spectrum collected, ideally, with no interaction with a sample; the variables in the equation are defined as in T1, with the exception of $S'(k)$, which is an example of $S(k)$ with no sample interaction with the beam.
Sources	[3, 5, 6]
Ref. By	T2

5.2.5 Instance Models

This section transforms the problem defined in Section 5.1 into one which is expressed in mathematical terms. It uses concrete symbols defined in Section 5.2.4 to replace the abstract symbols in the models identified in Sections 5.2.2 and 5.2.3.

The data processing goal GS2 is solved by the following instance models (IM1, IM2, IM3

IM4).

Number	IM1
Label	Normalization to the integral
Input	k_1 is the index of beginning of spectrum range (spectrum axis), user input k_2 is the index of end of spectrum range (spectrum axis), user input $I(E_k)$ is the 3D spectrum image, user input The input is constrained such that $k_1 \geq 0$, and $k_2 \leq N$
Output	$I_{norm}(E_k) = \frac{I(E_k)}{\sum_{E_k=k_1}^{E_k=k_2} I(E_k)}$
Description	$I(E_k)$ is a spectrum (DD1), user input k_1 : Index of beginning of spectrum range (spectrum axis), user input k_2 : Index of end of spectrum range (spectrum axis), user input K : Last index along the spectral axis x : Location along first spatial axis y : Location along second spatial axis $I_{norm}(E_k)$: Spectrum normalized along the spectral axis to the integral defined by a user Note that this algorithm can be applied to a 3D spectrum image (DD2) by applying the algorithm to each (x, y) pixel independently.
Sources	—
Ref. By	

Number	IM2
Label	Richardson-Lucy Deconvolution
Input	<p>$I_{PSF}(E)$ is the point spread function of the instrument (see DD3)</p> <p>$I_{real}^0(E)$ is the initial guess for the “real” spectrum (DD1)</p> <p>$I_{measured}(E)$ is the measured spectrum, as obtained from the spectrometer software (DD1)</p> <p>R is the total (non-negative integer) number of iterations of the deconvolution algorithm applied to the spectrum</p> <p>c is the number of the current iteration (at iteration 0, $c = 0$)</p> <p>i, j, l are each indices of pixels in the spectrum. Three different variables are used for the pixel index to make the effect of the summations clear.</p>
Equation	$I_{real(j)}^{c+1}(E) = I_{real(j)}^c(E) \sum_i \frac{I_{PSF}(E) I_{measured}(E)}{\sum_l I_{PSF}(E) I_{real(l)}^c(E)}, \text{ while } c < R$
Output	$I_{deconvolved}(E_k) = I_{real(j)}^R(E)$
Description	<p>The purpose of the RL deconvolution algorithm is to separate the effects of the spectrometer point spread function from the “real” signal of the sample. <i>I.e.</i> in T2, the signal is described as the convolution of the point spread function with the signal from the microscope. Deconvolution is usually run after normalization of the spectra IM1 to eliminate effects of changing beam current.</p> <p>This algorithm can also be expanded to apply to the 3D spectrum image (DD2)) by applying it at every (x, y) pixel in the spectrum image.</p>
Sources	[6, 7]
Ref. By	–

Number	IM3
Label	Background subtraction
Input	<p>$I_{collected}$ is the spectrum as collected by the spectrometer.</p> <p>$I_{background}(E)$ is a spectrum representing the background to be subtracted (this could be associated with the dark signal, or with the signal coming from unwanted, but unavoidable sources: <i>e.g.</i> outside noise, substrate signal...)</p>
Equation	$I_{sample} = I_{collected} - I_{background}$
Output	$I_{sample}(E)$
Description	<p>This model addresses the removal of background contributions to the signal ($b(k)$ in T1), where $b(k)$ is transformed to a spectrum (DD1) as a function of energy.</p> <p>The background spectrum must be of the same dimensions as the spectrum it is to be removed from. For the spectrum image, the background spectrum may be applied to each pixel.</p>
Sources	–
Ref. By	–

Number	IM4
Label	Gain correction
Input	<p>$I_{collected}$ is the spectrum (DD1) of the signal as collected by the spectrometer (see T1).</p> <p>$g(E)$ is the gain “spectrum” of the spectrometer $g(k)$ transformed into a function of energy (DD1)</p>
Equation	$I_{corrected}(E) = \frac{I_{collected}(E)}{g_E}$
Output	$I_{corrected}(E)$ is the spectrum after the gain correction from the spectrometer CCD is applied.
Description	This model addresses the removal of the gain ($g(k)$ in T1) from the collected signal, where $g(k)$ is transformed to a “spectrum” (DD1) as a function of energy.
Sources	–
Ref. By	–

5.2.6 Data Constraints

This section details the constraints on the data that the software must process, including the input, processing steps, and output from the software. Physical constraints based on the expectations of the dataset are left out to allow the user more freedom in the input.

- The input spectrum image (DD2) must be a 3D structure, or a 3D structure contained within a .dm3 or .h5 file;
- The user input number of iterations to use for the deconvolution algorithm must be an integer number greater than or equal to 0;
- For the normalization model, the user input of the number of bins to normalize must not be empty;
- The user input of the background signal (IM3) must be of the same length along the spectral axis as the spectrum image it will be applied to;
- The user input of the gain signal (IM4) must be of the same length along the spectral axis as the spectrum image it will be applied to;
- The normalization (IM1) and deconvolution (IM2) data processing algorithms both include a division by experimentally-derived values. The denominator in these steps must not be 0.

5.2.7 Properties of a Correct Solution

A correct solution must be acceptable to a user experienced with EELS and/or CL data processing, as is relevant to the EELS/CL data being processed.

6 Requirements

This section provides the functional requirements, the business tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is expected to exhibit.

6.1 Functional Requirements

R1: Accept and read the following as Spectrum Image inputs:

- 3D data array (eg, already stored in computer memory)
- File in format *.dm3 containing 3D data array
- File in format *.h5 containing 3D data array

R2: Accept and read the following as Spectrum inputs:

- 1D data array
- File containing 1D data array in *.csv format

R3: Verify that all data inputs are of the correct dimensionality and composed of Real numbers

R4: Accept user input to select a spectral range and extract (x,y) slices averaged over the selected spectral range and display the (x,y) slice as an image. The software should also export this image to an image file, as desired by the user.

R5: Accept user input to define an area on an (x,y) image display and extract a spectrum averaged over selected pixels. The software should also export this spectrum as a *.csv file, as desired by the user.

R6: Given a 1D spectrum array and an integer number, the software should perform that number of deconvolution iterations on a 3D EELS dataset using the 1D spectrum array as a reference of the system response. The software should display the output of the deconvolution for navigation by the user. Output of the deconvolution algorithm will be validated by an expert user.

R7: The software should be able to normalize a 3D spectrum image upon user command: either to an integrated portion of a chosen range along the spectral axis or to a single chosen channel.

R8: The software should be able to perform a background subtraction, given the appropriate inputs of a spectrum or spectrum image and a background reference spectrum.

R9: The software should be able to perform a gain correction, given the appropriate inputs of a spectrum or spectrum image and a gain reference spectrum.

6.2 Nonfunctional Requirements

The nonfunctional priorities for the software are the useability, speed, maintainability, expandability, and understandability. The user must be able to easily use the software to extract the data that they want and do the processing operations that they want, given the user characteristics defined elsewhere. In addition, a more advanced user may wish to add their own functions into the software data processing algorithms; the software should be written in such a way to make this simple and understandable. The speed of performance is of interest in the interactive display of the 3D datasets and in the data processing operations, which can be computationally heavy with large datasets. To improve the software over time and add new functionality as the data processing field expands, the software must be both maintainable and understandable by the original programmer and future programmers. A user may wish to perform their own tests of the software functions, emphasizing the need

to have transparent and understandable software. To reach a wide user base, the program should be usable on many different operating systems. The nonfunctional requirements are listed below:

- The software should be maintainable by the original programmer or future programmers to keep up to date with advances in data processing practices;
- The software should allow the addition of more data processing functions as required by an advanced user experienced in programming;
- The software should not display significant lag when interacting with the user, except in the case of data processing steps, which may be computationally expensive;
- Use of the interactive display and of data processing functions should be intuitive for a user experienced with the processing techniques for 3D datasets;
- The coding practices for the software should be open and transparent to facilitate inspection by an experienced user to encourage trust in the data processing steps performed;
- The display for the user to interact with should be readable: *i.e.* the text should be large enough to read by a user with average eyesight, with high contrast against the background for visibility;
- The colours used in the display should be clearly distinguishable from each other;
- The software should function on multiple operating systems, including Windows, Linux, and MacOS, in a laptop or desktop environment.

7 Likely Changes

This section details some changes which are likely to be made to the software once the initial requirements are met, in the interests of continuous improvement of the software's capabilities.

- LC1: A PSF unique to each pixel in the spectrum image (DD2) will be used instead of assuming one PSF is valid for all pixels within a spectrum image (A2)
- LC2: Cosmic rays appear as high intensity single pixel spikes in a spectrum and can be removed via 3D image filtering techniques. A future change will implement this filtering option for the user.

8 Traceability Matrices and Graphs

The purpose of the traceability matrices is to provide easy references on what has to be additionally modified if a certain component is changed. Every time a component is changed, the items in the column of that component that are marked with an “X” may have to be modified as well. Table 2 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 3 shows the dependencies of instance models, requirements, and data constraints on each other. Table 1 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

	A1	A2	A3	A4	A5
T1				X	X
T2	X		X		
GD1		X			
DD1	X				
DD2	X	X			
DD3	X	X			
IM1			X		
IM2	X	X			
IM3				X	
IM4					X

Table 1: Traceability Matrix Showing the Connections Between Assumptions and Other Items

	T1	T2	GD1	DD1	DD2	DD3	IM1	IM2	IM3	IM4
T1		X							X	X
T2										
GD1										
DD1	X								X	
DD2			X	X						
DD3	X			X				X		
IM1		X								
IM2	X	X				X				
IM3	X									
IM4	X									

Table 2: Traceability Matrix Showing the Connections Between Items of Different Sections

	IM1	IM2	IM3	IM4	5.2.6	R1	R2	R3	R4	R5	R6	R7	R8	R9
IM1						X						X		
IM2	X					X		X			X			
IM3						X	X	X					X	
IM4						X	X	X						X
R1					X	X		X		X				
R2					X			X			X			
R3					X	X	X		X	X			X	X
R4														
R5														
R6	X	X					X					X		
R7	X													
R8			X				X							
R9				X			X							

Table 3: Traceability Matrix Showing the Connections Between Requirements and Instance Models

References

- [1] W. S. Smith and L. Lai, “A new requirements template for scientific computing,” in *Proceedings of the First International Workshop on Situational Requirements Engineering Processes – Methods, Techniques and Tools to Support Situation-Specific Requirements Engineering Processes, SREP’05* (J. Ralyté, P. Ågerfalk, and N. Kraiem, eds.), (Paris, France), pp. 107–121, In conjunction with 13th IEEE International Requirements Engineering Conference, 2005.
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9 Appendix

[Your report may require an appendix. For instance, this is a good point to show the values of the symbolic parameters introduced in the report. —SS]

9.1 Symbolic Parameters

[The definition of the requirements will likely call for `SYMBOLIC_CONSTANTS`. Their values are defined in this section for easy maintenance. —SS]