Czerny-Turner Monochromator

This model simulates a grating spectrometer in a crossed Czerny-Turner configuration. The model uses the Geometrical Optics interface to compute the positions of incident rays on the detector plane, from which the instrument's spectral resolution can be derived.

Introduction

A Czerny-Turner spectrometer spatially separates polychromatic light into a series of monochromatic rays. The latter consists of a slit source, a spherical collimating mirror, a planar diffraction grating, a spherical imaging mirror, and an array charge coupled device (CCD) detector, see Figure 1.

With a given optical component arrangement and with the knowledge of the detector properties it is possible to determine the wavelength calibration as well as the spectral resolution of the instrument.

Model Definition

A Czerny-Turner spectrometer is usually designed with F-number > 3 to avoid large aberrations of the image at the detector. Accordingly, this model treats the polychromatic light source as a cone-based release of rays with F-number=10. Note that the system's F-number is related to its numerical aperture NA by:

$$\mathrm{F-number} = \frac{1}{2\mathrm{NA}}$$

Where the numerical aperture NA is related to the half-angle of the maximum cone of light that can enter the system Θ:

$$\mathrm{NA} = n\sin(\Theta)$$

Where n is the refractive index of the propagation medium (air, n=1).

The polychromatic source is simulated using twenty rays in frequency space that are sampled from a uniform distribution. The corresponding free-space wavelength distribution has a minimum of λ=451 nm and a maximum of λ=894 nm.

The geometry of the spectrometer is shown in Figure 1. The rays are released from the front focal point of the collimating mirror. The collimating mirror is tilted with an

angle θ_c to direct the collimated light toward the diffraction grating. The rays of diffraction order m=1 are then directed toward the focusing mirror; because the ray trajectories of nonzero diffraction order are frequency-dependent, the rays of different frequency arrive at the focusing mirror with different angles of incidence.

The focusing mirror reflects the rays onto the detector. The detector is composed of an array of N=3648 pixels of width w_p=8 μm. The geometrical parameters used in the model are listed in Table 1.

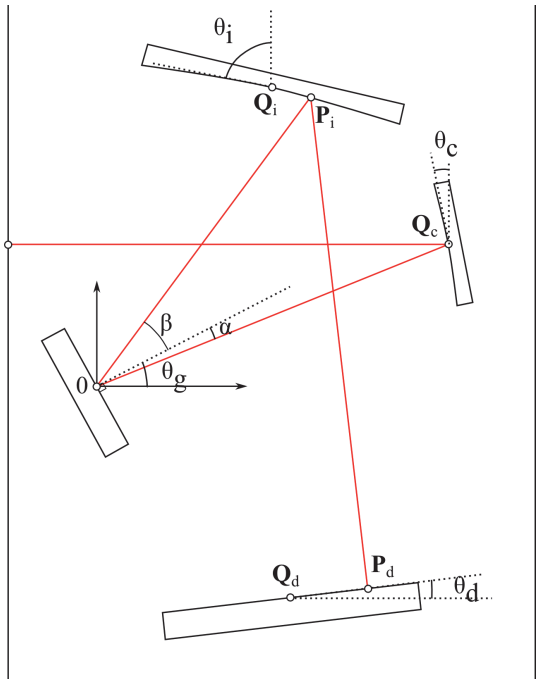

Figure 1: Typical crossed Czerny-Turner configuration. Numerical values are displayed in Table 1

TABLE 1: DEFINITION OF THE DESIGN PARAMETERS.

PARAMETERS	VALUE	DESCRIPTION
θ_g (deg)	28.76	Grating's angle
θ_c (deg)	11.0	Collimating mirror's angle
θ_i (deg)	77	Imaging mirror's angle
θ_d (deg)	6.76	Detector's angle
Q_i (mm)	(20.0,34.0)	Coordinates, imaging mirror

TABLE 1: DEFINITION OF THE DESIGN PARAMETERS.

PARAMETERS	VALUE	DESCRIPTION
Q_c (mm)	(40,16.161)	Coordinates, collimating mirror
Q_d (mm)	(22.08,-24.12)	Coordinates, detector
R_i (mm)	130	Radius of curvature, imaging mirror
R_c (mm)	100	Radius of curvature, collimating mirror

The ray trajectories can be used to compute the spectrometer's resolution. The pixel number p_{num} of a ray on the collector is

$$p_{\text{num}} = \text{ceil}\left(\frac{N}{2} - \frac{q_x - Q_{dx}}{w_p \cos(\theta_d)}\right)$$

Where N is the pixel number of the CCD, w_p the pixel's width, and q_x the x-coordinate of the particle hitting the detector. Q_{dx} and θ_d are respectively the detector's center x-coordinate and the angle of the CCD. The spectral (optical) resolution $\delta\lambda$ of the element can then be estimated by

$$\delta\lambda \propto \frac{\Delta\lambda}{N}\frac{w_i}{w_p}$$

Where $\Delta\lambda$=650 nm is the spectral range of the detector, and w_i is the width of the slit's image on the CCD.

The knowledge of the image width on the detector is made possible provided the distance between the two rays delimiting a pencil of rays of given wavelengths on the detector. Figure 2 shows how this distance is evaluated.

In Comsol, it is possible to evaluate the image width using the following expression:

```
gop.gopmaxop1(if(samefreq&&onccd,
gop.gopmaxop1(if(samefreq&&onccd,distance,0)),0))
```

where `gop.gopmaxop1` is an operator that returns the maximum value of an expression over all rays. The logical expression `samefreq&&onccd` is used to perform the maximum operator only over rays of a single frequency and to exclude rays other than those of diffraction order 0 that do not reach the CCD. These variables are defined as

```
samefreq=abs(gop.nu-dest(gop.nu))<1[Hz]
onccd=qx>0[mm]&&qx<40[mm]&&qy>-32[mm]&&qy<-15[mm]
```

Here the rectangle bounded by x=0, x=40 mm, y=-32 mm, and y=-15 mm is chosen because it encloses the CCD.

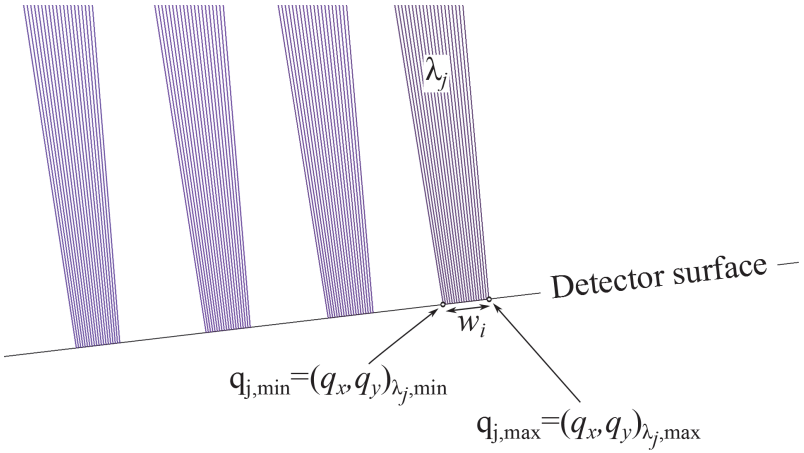

Figure 2: Determination of the image width for a given wavelength.

Results and Discussion

Figure 3 shows the ray trajectories in the spectrometer for a F-number of 10. The free-space wavelength is indicated by the color expression. After the rays are reflected by the grating, rays of different frequency propagate in different directions and arrive at different locations on the CCD. The pixel numbers corresponding to incident rays of each wavelength are plotted in Figure 4. The spectral resolution of the image is shown in Figure 5. The spectral resolution of a system determines the maximum number of spectral peaks that the spectrometer can resolve.

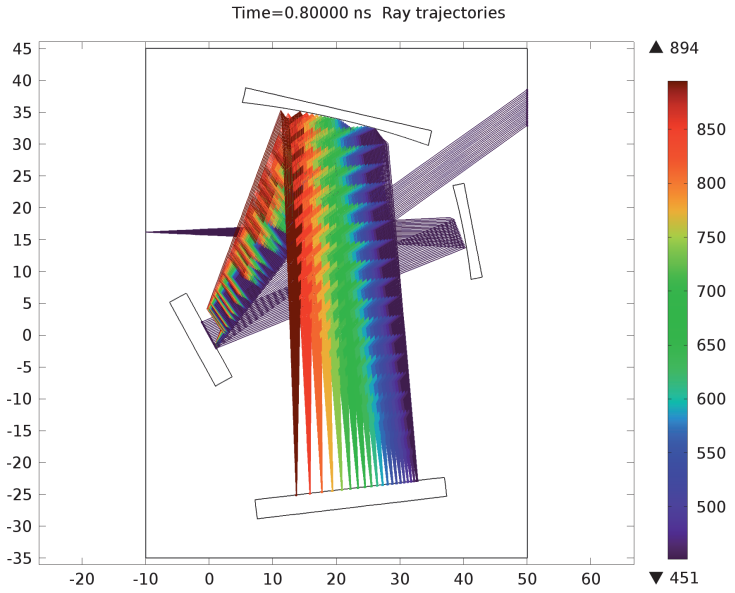

Figure 3: Wavelength separation on the CCD detector.

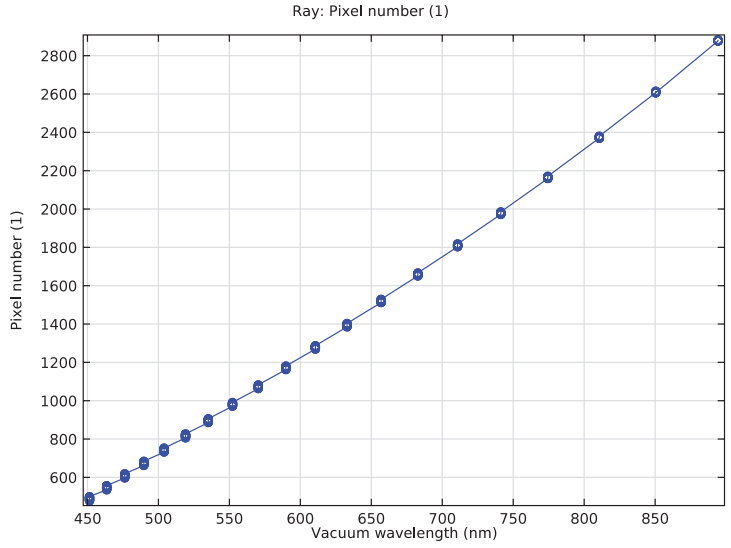

Figure 4: Wavelength calibration.

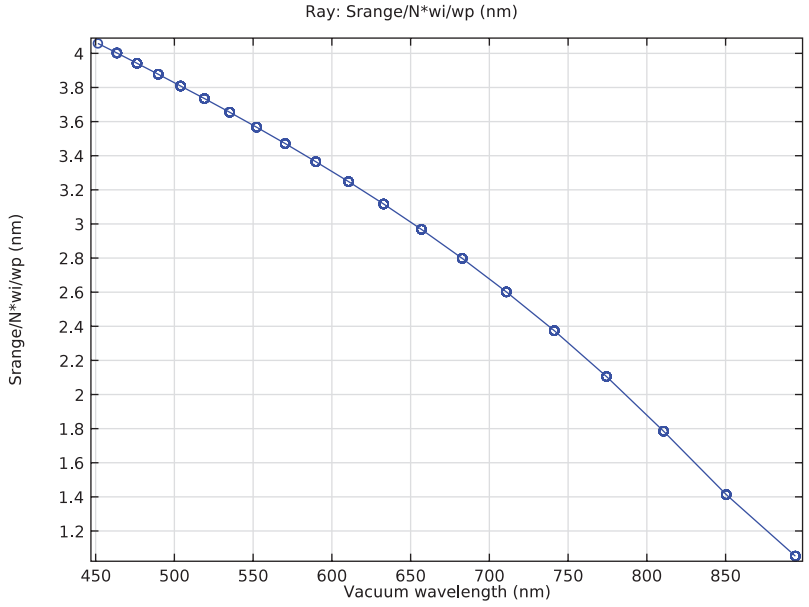

Figure 5: Spectral resolution as a function of the wavelength.

Reference

1. Liu K, Yu F; "Accurate wavelength calibration method using system parameters for grating spectrometers." Opt. Eng. vol. 52, no. 1, pp.013603-1—013603-6, 2013.

Model Library path: `Ray_Optics_Module/Polychromatic_Light/czerny_turner_monochromator`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

1 In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 In the **Select physics** tree, select **Optics>Ray Optics>Geometrical Optics (gop)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select study** tree, select **Preset Studies>Ray Tracing**.

6 Click **Done**.

GEOMETRY 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for Geometry, locate the **Units** section.

3 From the **Length unit** list, choose **mm**.

DEFINITIONS

Parameters

1 On the **Model** toolbar, click **Parameters**.

2 In the **Settings** window for Parameters, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Model Library folder and double-click the file `czerny_turner_monochromator_parameters.txt`.

GEOMETRY 1

Rectangle 1 (r1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

2 In the **Settings** window for Rectangle, locate the **Size** section.

3 In the **Width** text field, type `3`.

4 In the **Height** text field, type `15`.

5 Locate the **Position** section. From the **Base** list, choose **Center**.

6 In the **x** text field, type `-1.5*cos(theta_g)`.

7 In the **y** text field, type `-1.5*sin(theta_g)`.

8 Locate the **Rotation Angle** section. In the **Rotation** text field, type `theta_g`.

Rectangle 2 (r2)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

2 In the **Settings** window for Rectangle, locate the **Size** section.

3 In the **Width** text field, type `3`.

4 In the **Height** text field, type `15`.

5 Locate the **Position** section. From the **Base** list, choose **Center**.

6 In the **x** text field, type `Qcx`.

7 In the **y** text field, type `Qcy`.

8 Locate the **Rotation Angle** section. In the **Rotation** text field, type `theta_c`.

Circle 1 (c1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Circle**.

2 In the **Settings** window for Circle, locate the **Size and Shape** section.

3 In the **Radius** text field, type `Rc`.

4 Locate the **Position** section. In the **x** text field, type `Qcx-Rc*cos(theta_c)`.

5 In the **y** text field, type `Qcy-Rc*sin(theta_c)`.

Difference 1 (dif1)

1 On the **Geometry** toolbar, click **Booleans and Partitions** and choose **Difference**.

2 Click the **Zoom Extents** button on the **Graphics** toolbar.

3 Select the object **r2** only.

4 In the **Settings** window for Difference, locate the **Difference** section.

5 Find the **Objects to subtract** subsection. Select the **Active** toggle button.

6 Select the object **c1** only.

Rectangle 3 (r3)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

2 In the **Settings** window for Rectangle, locate the **Size** section.

3 In the **Width** text field, type `3`.

4 In the **Height** text field, type `30`.

5 Locate the **Position** section. From the **Base** list, choose **Center**.

6 In the **x** text field, type `Qix`.

7 In the **y** text field, type `Qiy`.

8 Locate the **Rotation Angle** section. In the **Rotation** text field, type `theta_i`.

Circle 2 (c2)

1 On the **Geometry** toolbar, click **Primitives** and choose **Circle**.

2 In the **Settings** window for Circle, locate the **Size and Shape** section.

3 In the **Radius** text field, type `Ri`.

4 Locate the **Position** section. In the **x** text field, type `Qix-Ri*cos(theta_i)`.

5 In the **y** text field, type `Qiy-Ri*sin(theta_i)`.

Difference 2 (dif2)

1 On the **Geometry** toolbar, click **Booleans and Partitions** and choose **Difference**.

2 Select the object **r3** only.

3 In the **Settings** window for Difference, locate the **Difference** section.

4 Find the **Objects to subtract** subsection. Select the **Active** toggle button.

5 Select the object **c2** only.

Rectangle 4 (r4)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

2 In the **Settings** window for Rectangle, locate the **Size** section.

3 In the **Width** text field, type `30`.

4 In the **Height** text field, type `3`.

5 Locate the **Position** section. From the **Base** list, choose **Center**.

6 In the **x** text field, type `Qdx+1.5*sin(theta_d)`.

7 In the **y** text field, type `Qdy-1.5*cos(theta_d)`.

8 Locate the **Rotation Angle** section. In the **Rotation** text field, type `theta_d`.

Rectangle 5 (r5)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

2 In the **Settings** window for Rectangle, locate the **Size** section.

3 In the **Width** text field, type `60`.

4 In the **Height** text field, type `80`.

5 Locate the **Position** section. In the **x** text field, type `-10`.

6 In the **y** text field, type `-35`.

7 Click the **Build All Objects** button.

8 Click the **Zoom Extents** button on the **Graphics** toolbar.

GEOMETRICAL OPTICS (GOP)

Select the **Frequency-dependent refractive indices** check box to release a distribution of rays of different free-space wavelengths. Also, increase the maximum number of secondary rays to 1200.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometrical Optics (gop)**.
2 In the **Settings** window for Geometrical Optics, locate the **Advanced Settings** section.
3 Select the **Frequency-dependent refractive indices** check box.
4 In the **Maximum number of secondary rays** text field, type 1200.
5 Select Domain 1 only.

Medium Properties 1

1 On the **Physics** toolbar, click **Global** and choose **Release from Grid**.

Release rays from a grid point located at the focus of the collimating mirror. Use a cone angle that corresponds to the numerical aperture of the system and select a uniform frequency distribution for the initial rays.

Release from Grid 1

1 In the **Settings** window for Release from Grid, locate the **Initial Coordinates** section.
2 In the $q_{x,0}$ text field, type `-10`.
3 In the $q_{y,0}$ text field, type `16.16104903340627`.
4 Locate the **Ray Direction Vector** section. From the **Ray direction vector** list, choose **Conical**.
5 In the N_w text field, type `20`.
6 In the α text field, type `asin(NA)`.
7 Locate the **Initial Ray Frequency** section. From the **Distribution function** list, choose **Uniform**.
8 In the N text field, type `20`.
9 In the μ text field, type `c_const/lam`.
10 In the σ text field, type `0.2*c_const/lam`.
11 On the **Physics** toolbar, click **Boundaries** and choose **Wall**.

Select the **Bounce** wall condition for the curved mirrors.

Wall 2

1 In the **Settings** window for Wall, locate the **Wall Condition** section.

2 From the **Wall condition** list, choose **Bounce**.

3 Select Boundaries 19 and 20 only.

4 On the **Physics** toolbar, click **Boundaries** and choose **Grating**.

Add a grating with a groove density of 600 lines/mm and include the first diffraction order. Note that in grating spectrometer systems, the first order spectra usually carry the primary diffraction intensity of the grating.

Grating 1

1 Select Boundary 6 only.

2 In the **Settings** window for Grating, locate the **Device Properties** section.

3 In the d text field, type `1[mm]/600`.

4 On the **Physics** toolbar, click **Attributes** and choose **Diffraction Order**.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for Mesh, locate the **Mesh Settings** section.

3 From the **Sequence type** list, choose **User-controlled mesh**.

Refine the mesh around the curved surfaces.

Size

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.

2 In the **Settings** window for Size, locate the **Element Size** section.

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Minimum element size** text field, type `0.002`.

5 In the **Curvature factor** text field, type `0.002`.

6 Click the **Build All** button.

DEFINITIONS

Add the definition for the pixel number and for the image width of the entrance slit. The latter expression uses the `maxop` operator, if conditions and the `dest` operator to determine the difference in position of extremum rays for a given wavelength.

1 In the **Model Builder** window, expand the **Study 1** node.

Variables 1

1 Right-click **Component 1 (comp1)>Definitions** and choose **Variables**.

2 In the **Settings** window for Variables, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
pnum	ceil(N/2-(qx-Qdx)/(wp*cos(theta_d)))		Pixel number
wi	gop.gopmaxop1(if(samefreq&&onccd,gop.gopmaxop1(if(samefreq&&onccd,distance,0)),0))	m	Image width of the entrance slit
samefreq	abs(gop.nu-dest(gop.nu))<1[Hz]		Are rays of same frequency?
onccd	qx>0[mm]&&qx<40[mm]&&qy>-32[mm]&&qy<-15[mm]		Are rays close to the detector?
distance	sqrt((qx-dest(qx))^2+(qy-dest(qy))^2)	m	Distance between the rays

STUDY 1

Step 1: Ray Tracing

1 In the **Model Builder** window, under **Study 1** click **Step 1: Ray Tracing**.

2 In the **Settings** window for Ray Tracing, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,0.01,0.8)`.

4 On the **Model** toolbar, click **Compute**.

RESULTS

Data Sets

1 In the **Model Builder** window, expand the **Results>Data Sets** node.

2 Right-click **Ray 1** and choose **Duplicate**.

3 On the **Results** toolbar, click **Selection**.

4 In the **Settings** window for Selection, locate the **Geometric Entity Selection** section.

5 From the **Geometric entity level** list, choose **Boundary**.

6 Select Boundary 11 only.

Ray Trajectories (gop)

1 In the **Model Builder** window, expand the **Results>Ray Trajectories (gop)>Ray Trajectories 1** node, then click **Color Expression 1**.

2 In the **Settings** window for Color Expression, locate the **Expression** section.

3 In the **Expression** text field, type `gop.lambda0`.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Spectrum**.

5 Locate the **Expression** section. From the **Unit** list, choose **nm**.

6 On the **2D plot group** toolbar, click **Plot**.

Compare the resulting plot to Figure 3.

1D Plot Group 2

1 On the **Model** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for 1D Plot Group, locate the **Data** section.

3 From the **Data set** list, choose **Ray 2**.

4 From the **Time selection** list, choose **Last**.

5 On the **1D plot group** toolbar, click **Ray**.

6 In the **Settings** window for Ray, locate the **y-Axis Data** section.

7 In the **Expression** text field, type `pnum`.

8 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

9 In the **Expression** text field, type `gop.lambda0`.

10 From the **Unit** list, choose **nm**.

11 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

12 From the **Positioning** list, choose **In data points**.

13 On the **1D plot group** toolbar, click **Plot**.

Compare the resulting plot to Figure 4.

1D Plot Group 3

1 On the **Model** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for 1D Plot Group, locate the **Data** section.

3 From the **Data set** list, choose **Ray 2**.

4 From the **Time selection** list, choose **Last**.

5 On the **1D plot group** toolbar, click **Ray**.

6 In the **Settings** window for Ray, locate the **y-Axis Data** section.

7 In the **Expression** text field, type `Srange/N*wi/wp`.

8 From the **Unit** list, choose **nm**.

9 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

10 In the **Expression** text field, type `gop.lambda0`.

11 From the **Unit** list, choose **nm**.

12 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

13 From the **Positioning** list, choose **In data points**.

14 On the **1D plot group** toolbar, click **Plot**.

Compare the resulting plot to Figure 5.