Created in COMSOL Multiphysics 6.1



# Czerny-Turner Monochromator

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## Introduction

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.

A Czerny-Turner spectrometer spatially separates polychromatic light into a series of monochromatic rays. The configuration includes 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:

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

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

$$NA = n \sin(\Theta)$$

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

The polychromatic source is simulated using twenty frequency values that are sampled from a uniform distribution. The corresponding free-space wavelength distribution has a minimum of  $\lambda$ =460 nm and a maximum of  $\lambda$ =840 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  $\theta_c$  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 at different positions and 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  $w_p = 8 \ \mu\text{m}$ . 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

PARAMETERS	VALUE	DESCRIPTION
$\theta_g$ (deg)	28.76	Grating's angle
$\theta_c ~({\rm deg})$	11.0	Collimating mirror's angle
$\theta_i$ (deg)	77	Imaging mirror's angle
$\theta_d$ (deg)	6.76	Detector's angle
$Q_i$ (mm)	(20.0,34.0)	Coordinates, imaging mirror
$Q_c$ (mm)	(40,16.161)	Coordinates, collimating mirror
$Q_d$ (mm)	(22.08,-24.12)	Coordinates, detector

TABLE I: DEFINITION OF THE DESIGN PARAMETERS.

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PARAMETERS	VALUE	DESCRIPTION
$R_i$ (mm)	130	Radius of curvature, imaging mirror
$R_c~({ m mm})$	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

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

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  $\theta_d$  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 given by the distance between the two rays delimiting a pencil of rays of uniform wavelength on the detector. Figure 2 shows how this distance is evaluated.

It is possible to evaluate the image width using the following expression:

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

where gop.gopmaxop1 is a nonlocal coupling that returns the maximum value of an expression over all rays. Two nested maximum couplings are used because the resulting width should be the maximum distance from any ray to any other ray of the same frequency. The logical expression samefreq is used to evaluate the maximum only over rays of a single frequency. This variable is defined as

samefreq=abs(gop.nu-dest(gop.nu))<1[Hz]</pre>



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

## Results and Discussion

Figure 3 shows the ray trajectories in the spectrometer for an F-number of 10. The freespace 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. K. Liu and F. Yu, "Accurate wavelength calibration method using system parameters for grating spectrometers," *Opt. Eng.*, vol. 52, no. 1, pp. 013603-1–013603-6, 2013.

## Application Library path: Ray\_Optics\_Module/ Spectrometers\_and\_Monochromators/czerny\_turner\_monochromator

## Modeling Instructions

From the File menu, choose New.

NEW In the New window, click Solution Model Wizard.

## MODEL WIZARD

- I 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  $\bigcirc$  Study.
- 5 In the Select Study tree, select Preset Studies for Selected Physics Interfaces>Ray Tracing.
- 6 Click M Done.

#### ROOT

Insert the prepared geometry sequence from file. You can read the instructions for creating the geometry in the appendix.

### GEOMETRY I

- I In the Geometry toolbar, click Insert Sequence and choose Insert Sequence.
- 2 Browse to the model's Application Libraries folder and double-click the file czerny\_turner\_monochromator\_geom\_sequence.mph.
- 3 In the Geometry toolbar, click 🟢 Build All.
- **4** Click the **Zoom Extents** button in the **Graphics** toolbar.

## GLOBAL DEFINITIONS

Parameters 1

- I In the Model Builder window, under Global Definitions click Parameters I.
- 2 In the Settings window for Parameters, locate the Parameters section.
- **3** In the table, enter the following settings:

Name	Expression	Value	Description
lambda0min	450[nm]	4.5E-7 m	Minimum vacuum wavelength
lambda0max	850[nm]	8.5E-7 m	Maximum vacuum wavelength
Ν	3648	3648	Number of pixels
wp	8[um]	8E-6 m	Pixel width
Fnum	10	10	F-number
NA	1/(2*Fnum)	0.05	Numerical aperture
Srange	650[nm]	6.5E-7 m	Spectral range

#### **GEOMETRICAL OPTICS (GOP)**

- I In the Model Builder window, under Component I (compl) click Geometrical Optics (gop).
- 2 In the Settings window for Geometrical Optics, locate the Domain Selection section.
- 3 Click Clear Selection.
- 4 Locate the Ray Release and Propagation section. From the Wavelength distribution of released rays list, choose Polychromatic, specify vacuum wavelength.

#### Release from Grid I

I In 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.

- 2 In the Settings window for Release from Grid, locate the Initial Coordinates section.
- **3** In the  $q_{x,0}$  text field, type -10.
- **4** In the  $q_{y,0}$  text field, type 16.16104903340627.
- 5 Locate the Ray Direction Vector section. From the Ray direction vector list, choose Conical.
- **6** In the  $N_{\rm w}$  text field, type 20.
- 7 In the  $\alpha$  text field, type asin(NA).
- 8 Locate the Vacuum Wavelength section. From the Distribution function list, choose Uniform.
- **9** In the N text field, type 20.
- **IO** In the  $\lambda_{0,\min}$  text field, type lambdaOmin.

II In the  $\lambda_{0,max}$  text field, type lambda0max.

## Wall I

- I In the Physics toolbar, click Boundaries and choose Wall.
- **2** Select Boundary 8 only.

#### Mirror I

- I In the Physics toolbar, click Boundaries and choose Mirror.
- **2** Select Boundaries 15 and 16 only.

## Grating I

I In 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.

- **2** Select Boundary **3** only.
- 3 In the Settings window for Grating, locate the Device Properties section.
- 4 In the d text field, type 1[mm]/600.
- 5 From the Rays to release list, choose Reflected.
- 6 Locate the Grating Orientation section. From the Direction of periodicity list, choose Reverse.

Diffraction Order (m = 0)

- In the Model Builder window, expand the Grating I node, then click
   Diffraction Order (m = 0).
- 2 In the Settings window for Diffraction Order, locate the Device Properties section.
- **3** In the *m* text field, type 1.

## MESH I

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 2 In the Settings window for Mesh, locate the Sequence Type section.
- 3 From the list, choose User-controlled mesh.

Refine the mesh around the curved surfaces.

#### Size

- I In the Model Builder window, under Component I (compl)>Mesh I 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 📗 Build All.

## DEFINITIONS

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

#### Variables I

- I In the Model Builder window, under Component I (compl) right-click Definitions and choose Variables.
- 2 In the Settings window for Variables, locate the Variables section.

Name	Expression	Unit	Description
pnum	<pre>ceil(N/2-(qx-Qdx)/(wp* cos(theta_d)))</pre>		Pixel number
samefreq	abs(gop.nu-dest(gop.nu))<1[Hz]		Logical expression for rays on the detector with the same frequency
distance	<pre>sqrt((qx-dest(qx))^2+(qy- dest(qy))^2)</pre>	m	Distance between the rays
distance2	<pre>gop.max(if(samefreq,distance,0))</pre>	m	Maximum distance to given ray
wi	<pre>gop.max(if(samefreq,distance2, 0))</pre>	m	Image width of the entrance slit

**3** In the table, enter the following settings:

#### STUDY I

Step 1: Ray Tracing

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

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

**3** In the **Output times** text field, type range(0,0.01,0.8).

**4** In the **Home** toolbar, click **= Compute**.

## RESULTS

#### Ray Bin I

- I In the Model Builder window, expand the Results>Datasets node.
- 2 Right-click Results>Datasets and choose More Datasets>Ray Bin.
- In the Settings window for Ray Bin, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)>
   Geometrical Optics>Ray properties>gop.lambda0 Vacuum wavelength m.
- 4 Locate the Bins section. From the Entry method list, choose Tolerance.
- **5** In the **Tolerance** text field, type 1[nm].

#### Ray Trajectories I

- I In the Model Builder window, expand the Results>Ray Trajectories (gop) node, then click Ray Trajectories I.
- 2 In the Settings window for Ray Trajectories, locate the Coloring and Style section.
- 3 Find the Line style subsection. From the Type list, choose Tube.
- 4 Select the Radius scale factor check box. In the associated text field, type 0.025.

#### Color Expression 1

- I In the Model Builder window, expand the Ray Trajectories I node, then click Color Expression I.
- 2 In the Settings window for Color Expression, click Replace Expression in the upper-right corner of the Expression section. From the menu, choose Component I (compl)> Geometrical Optics>Ray properties>gop.lambda0 Vacuum wavelength m.
- 3 Locate the Coloring and Style section. Click Change Color Table.
- 4 In the Color Table dialog box, select Rainbow>Spectrum in the tree.
- 5 Click OK.
- 6 In the Settings window for Color Expression, locate the Expression section.
- 7 From the Unit list, choose nm.
- 8 In the Ray Trajectories (gop) toolbar, click 🗿 Plot.
- 9 Click the Zoom Extents button in the Graphics toolbar. Compare the resulting plot to Figure 3.

#### Pixel Number

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Pixel Number in the Label text field.

- 3 Locate the Data section. From the Dataset list, choose Ray Bin I.
- 4 From the Time selection list, choose Last.

#### Ray I

- I In the Pixel Number toolbar, click  $\sim$  More Plots and choose Ray.
- 2 In the Settings window for Ray, locate the y-Axis Data section.
- 3 In the Expression text field, type pnum.
- 4 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 5 In the Expression text field, type gop.lambda0.
- 6 From the Unit list, choose nm.
- 7 Click to expand the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.
- 8 In the Pixel Number toolbar, click 💿 Plot. Compare the resulting plot to Figure 4.

#### Device Resolution

- I In the Home toolbar, click 🚛 Add Plot Group and choose ID Plot Group.
- 2 In the Settings window for ID Plot Group, type Device Resolution in the Label text field.
- 3 Locate the Data section. From the Dataset list, choose Ray Bin I.
- 4 From the Time selection list, choose Last.
- 5 Click to expand the Title section. From the Title type list, choose None.

#### Ray I

- I In the Device Resolution toolbar, click  $\sim$  More Plots and choose Ray.
- 2 In the Settings window for Ray, locate the y-Axis Data section.
- 3 In the Expression text field, type Srange/N\*wi/wp.
- 4 From the Unit list, choose nm.
- **5** Select the **Description** check box. In the associated text field, type **Spectral** resolution.
- 6 Locate the x-Axis Data section. From the Parameter list, choose Expression.
- 7 In the **Expression** text field, type gop.lambda0.
- 8 From the Unit list, choose nm.
- **9** Locate the **Coloring and Style** section. Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.
- **IO** In the **Device Resolution** toolbar, click **IO Plot**. Compare the resulting plot to Figure 5.

## ADD COMPONENT

In the Home toolbar, click  $\bigotimes$  Add Component and choose 2D.

## GEOMETRY I

I In the Settings window for Geometry, locate the Units section.

2 From the Length unit list, choose mm.

## GLOBAL DEFINITIONS

#### Parameters 1

I In the Model Builder window, under Global Definitions click Parameters I.

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

**3** In the table, enter the following settings:

Name	Expression	Value	Description
theta_g	28.76[deg]	0.50196 rad	Grating's angle
theta_c	11[deg]	0.19199 rad	Collimating mirror's angle
theta_i	77[deg]	1.3439 rad	Imaging mirror's angle
theta_d	6.76[deg]	0.11798 rad	Detector's angle
Qix	20[mm]	0.02 m	x coordinate Qi
Qiy	34[mm]	0.034 m	y coordinate Qi
Qcx	40[mm]	0.04 m	x coordinate Qc
Qcy	40*tan(2*theta_c)	16.161	y coordinate Qc
Qdx	22.08[mm]	0.02208 m	x coordinate Qd
Qdy	-24.12[mm]	-0.02412 m	y coordinate Qd
Ri	130[mm]	0.13 m	Imaging mirror's radius of curvature
Rc	100[mm]	0.1 m	Collimating mirror's radius of curvature

## GEOMETRY I

Rectangle 1 (r1)

I In the **Geometry** toolbar, click Rectangle.

- 2 In the Settings window for Rectangle, locate the Size and Shape 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)

- I In the Geometry toolbar, click 📃 Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape 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 I (c1)

- I In the **Geometry** toolbar, click 🕑 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 I (dif1)

- I In the Geometry toolbar, click i Booleans and Partitions and choose Difference.
- **2** Click the  $4 \rightarrow$  **Zoom Extents** button in 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. Click to select the **Selection** toggle button.
- **6** Select the object **c1** only.

## Rectangle 3 (r3)

- I In the **Geometry** toolbar, click **Rectangle**.
- 2 In the Settings window for Rectangle, locate the Size and Shape 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)

- I In the **Geometry** toolbar, click (•) **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)

- I In 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. Click to select the **CAL Activate Selection** toggle button.
- **5** Select the object **c2** only.

#### Rectangle 4 (r4)

- I In the **Geometry** toolbar, click **Rectangle**.
- 2 In the Settings window for Rectangle, locate the Size and Shape 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.

9 Click 🟢 Build All Objects.

**IO** Click the **Com Extents** button in the **Graphics** toolbar.