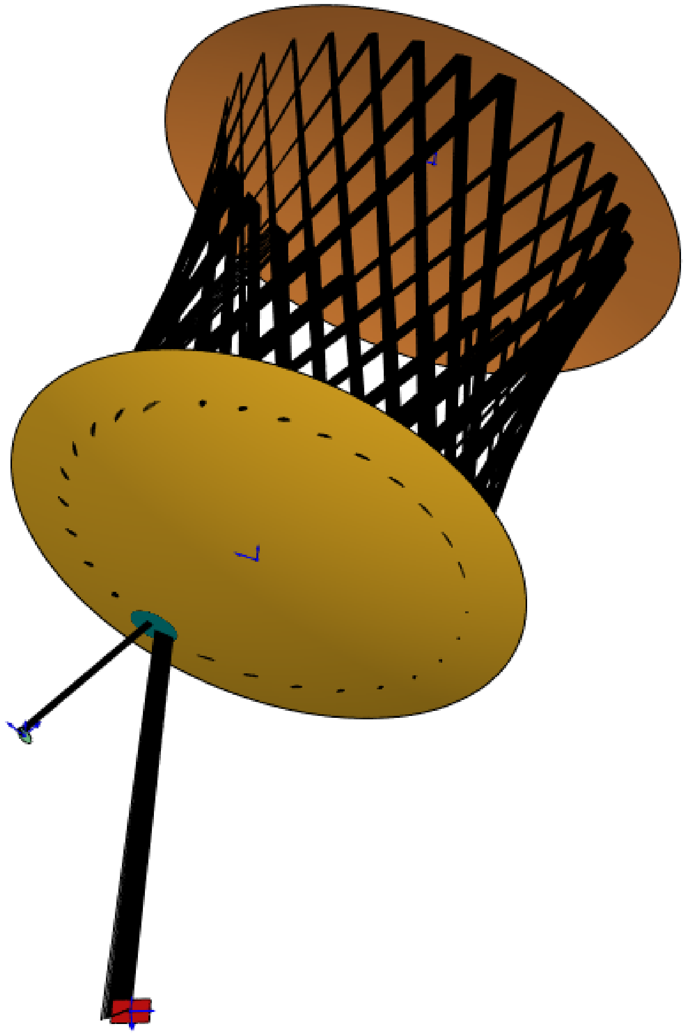
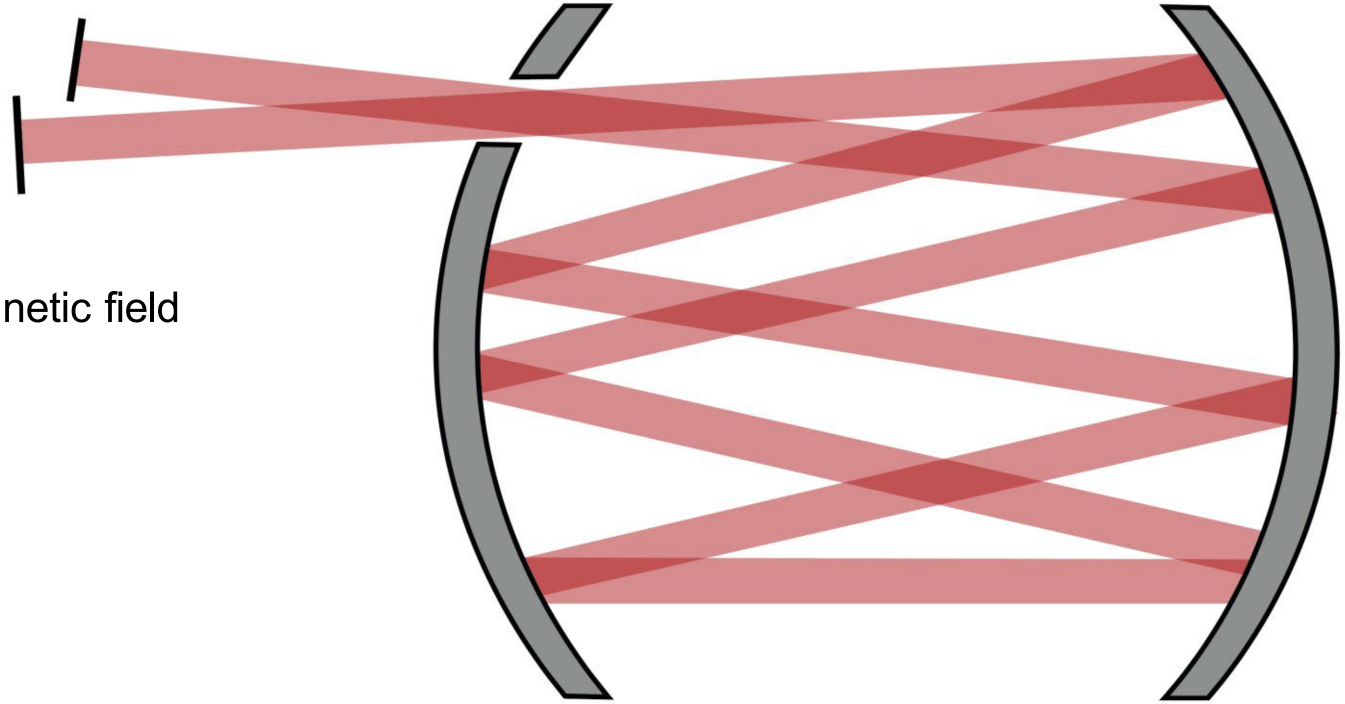
Modeling of a Herriott Cell

Abstract



In spectroscopy of gases, in order to obtain a sensitive enough measurement of the absorption, it is often required to have long optical path lengths. Multiple-pass cells, where the gas-filled volume is encased between mirrors, are a way of fulfilling this requirement while at the same time controlling beam divergence on the way and preempting the need for extremely large devices. The Herriott cell is one example of this kind of system, characterized by the use of two spherical mirrors with a single off-axis hole drilled into one of them to allow for the entry and exit of the beam. The curvature of the mirrors redirects the beam and controls its divergence. In this use case, we investigate the simulation of a Herriott cell with the optics modeling and design software VirtualLab Fusion.

Task Description



Gaussian wave

- 2 µm central wavelength
- 250 µm × 250 µm waist diameter

detector

electromagnetic field

Herriott cell

- 100 mm radius of curvature
- 2.5 mm × 2.5 mm hole
- Filled with:
  - air
  - CO_2* (n=1.00044, absorption coefficient 0.1 1/m)

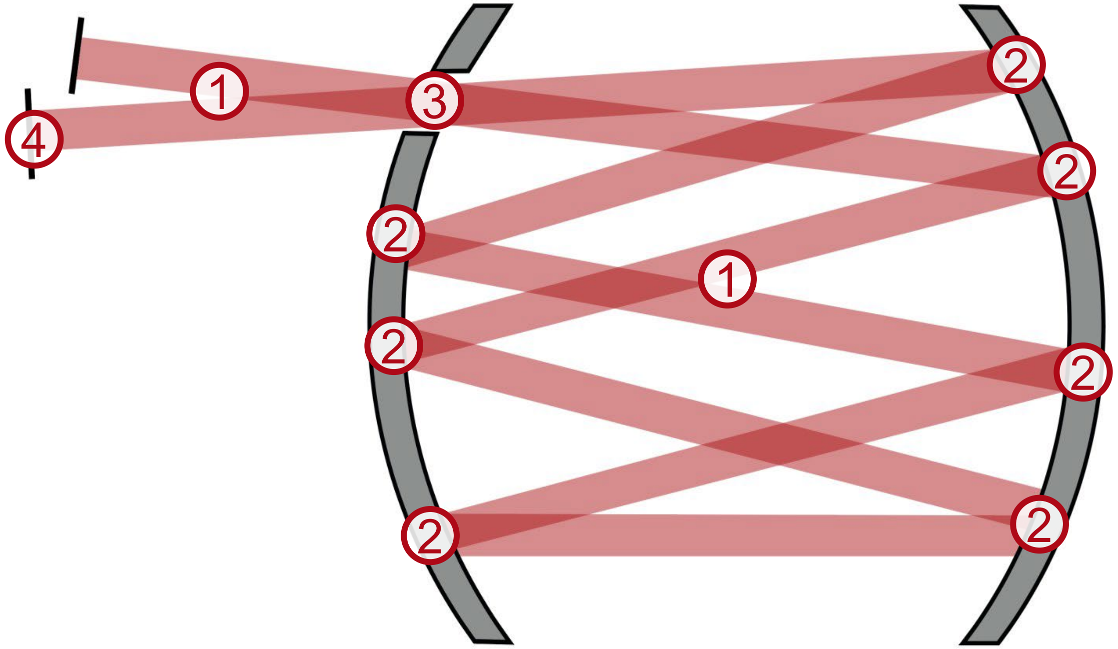
** Values from:*

- *Old, J. G., K. L. Gentili, and E. R. Peck. "Dispersion of carbon dioxide." JOSA 61.1 (1971): 89-90.*
- *Wei, Peng-Sheng, et al. "Absorption coefficient of carbon dioxide across atmospheric troposphere layer." Heliyon 4.10 (2018): e00785.*

Single-Platform Interoperability of Modeling Techniques

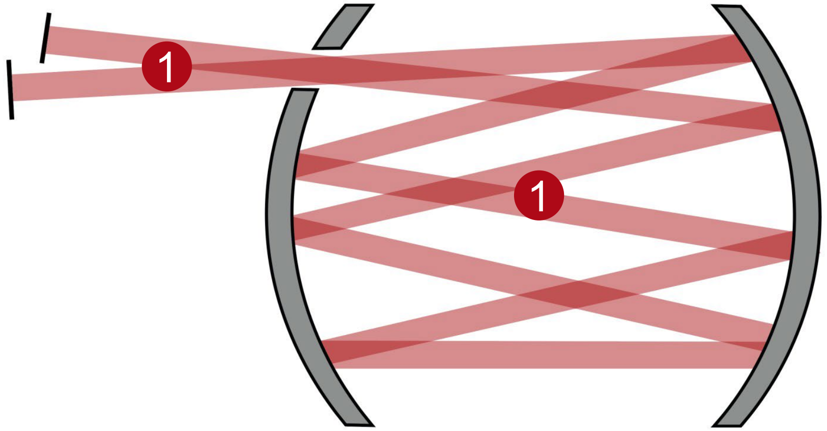
Each beam interacts with very different kinds of optical components while propagating through the complex system. Therefore, an accurate model requires a seamless interoperability of algorithms to be able to handle all aspects that arise:

① free-space propagation
② reflection at the mirrors of the cell
③ propagation through the hole
④ detector



Connected Modeling Techniques: Free-Space Propagation

① free-space propagation
② reflection at the mirrors of the cell
③ propagation through the hole
④ detector



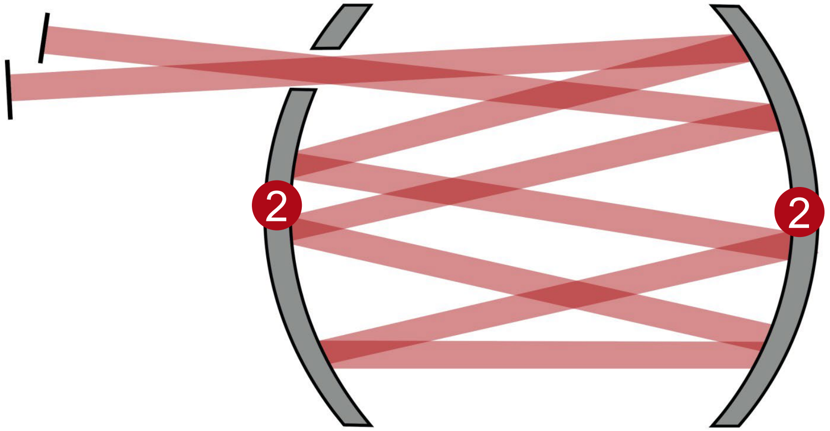
Available modeling techniques for free-space propagation:

Methods	Preconditions	Accuracy	Speed	Comments
Rayleigh Sommerfeld Integral	None	High	Low	Rigorous solution
Fourier Domain Techniques	None	High	High	Rigorous mathematical reformulation of RS integral
Fresnel Integral	**Paraxial**	High	High	Assumes paraxial light; moderate speed for very short distances
	Non-paraxial	Low	High	
Geometric Propagation	**Low diffraction**	High	Very high	Neglects diffraction effects
	Otherwise	Low	Very high	

In this particular case diffraction effects can be neglected as there are no hard edges or strong aperture effects. With this in mind, **Geometric Propagation** was chosen for a fast simulation of the system

Connected Modeling Techniques: Mirrors

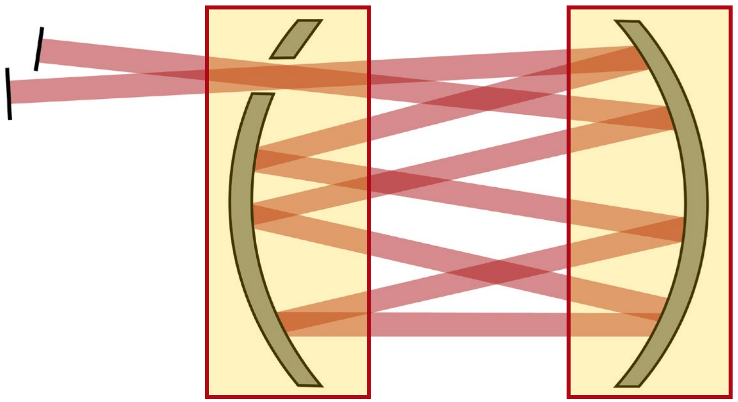
① free-space propagation
② reflection at the mirrors of the cell
③ propagation through the hole
④ detector



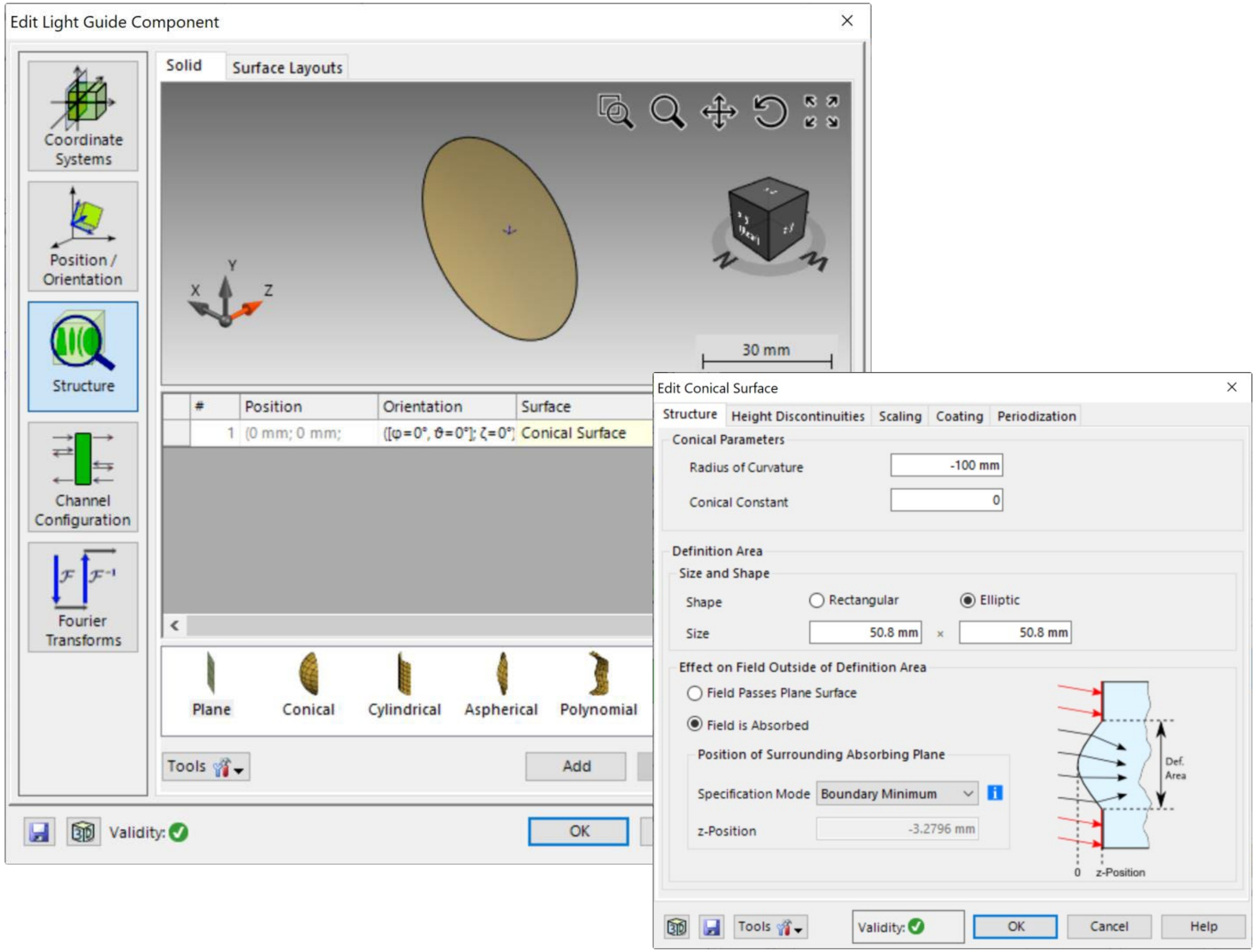
Methods	Preconditions	Accuracy	Speed	Comments
Functional Approach	No Fresnel losses	Low	Very High	Idealized version of a mirror
S matrix	Planar surface	High	High	Rigorous model; includes evanescent waves (for e.g. FTIR effect modeling)
Local Planar Interface Approximation	Surface not in focal region of beam	High	High	Local application of S matrix; LPIA; x-domain

In the case of the Herriott Cell we must deal with curved surfaces and have no focal regions in the system. Hence, the **Local Planar Interface Approximation (LPIA)** offers optimal speed and accuracy characteristics.

Conical Mirrors



In the *Light Guide Component*, it is possible to define regions on surfaces where a modeling technique different from that of the rest of the interface is applied. We use this feature to model the hole drilled in the first mirror of the cell to allow the entry and exit of the beam. To simulate the spherical shape of the mirror we select a *Conical Surface* with conical constant 0.



#	Position	Orientation	Surface
1	(0 mm; 0 mm;	([φ=0°, ϑ=0°]; ζ=0°)	Conical Surface

Edit Conical Surface

Conical Parameters

Radius of Curvature: -100 mm

Conical Constant: 0

Definition Area

Size and Shape

Shape: ○ Rectangular ● Elliptic

Size: 50.8 mm × 50.8 mm

Effect on Field Outside of Definition Area

○ Field Passes Plane Surface

● Field is Absorbed

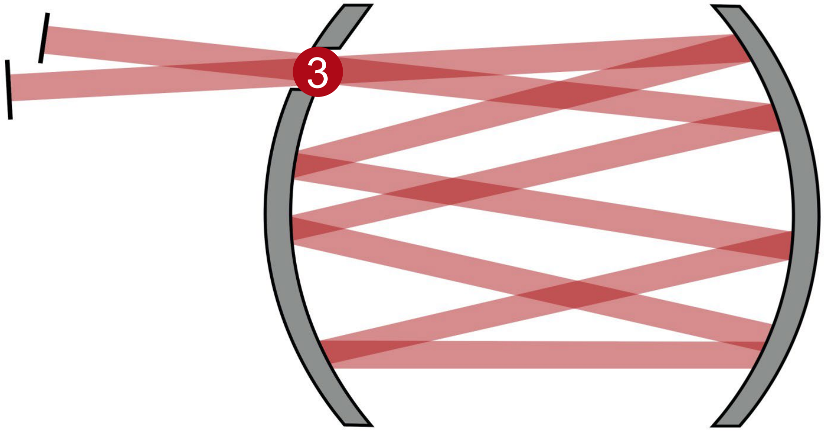
Position of Surrounding Absorbing Plane

Specification Mode: Boundary Minimum

z-Position: -3.2796 mm

Connected Modeling Techniques: Hole

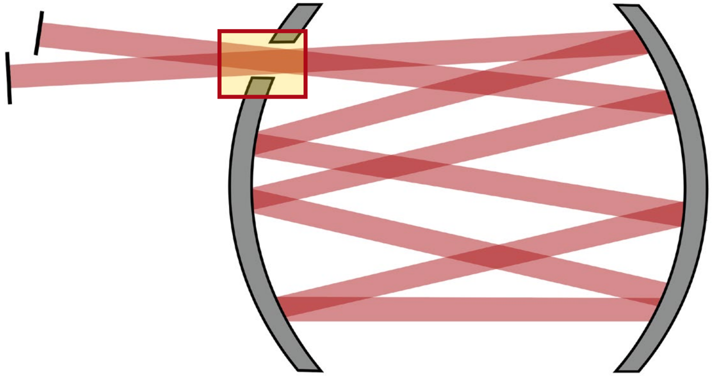
① free-space propagation
② reflection at the mirrors of the cell
③ propagation through the hole
④ detector



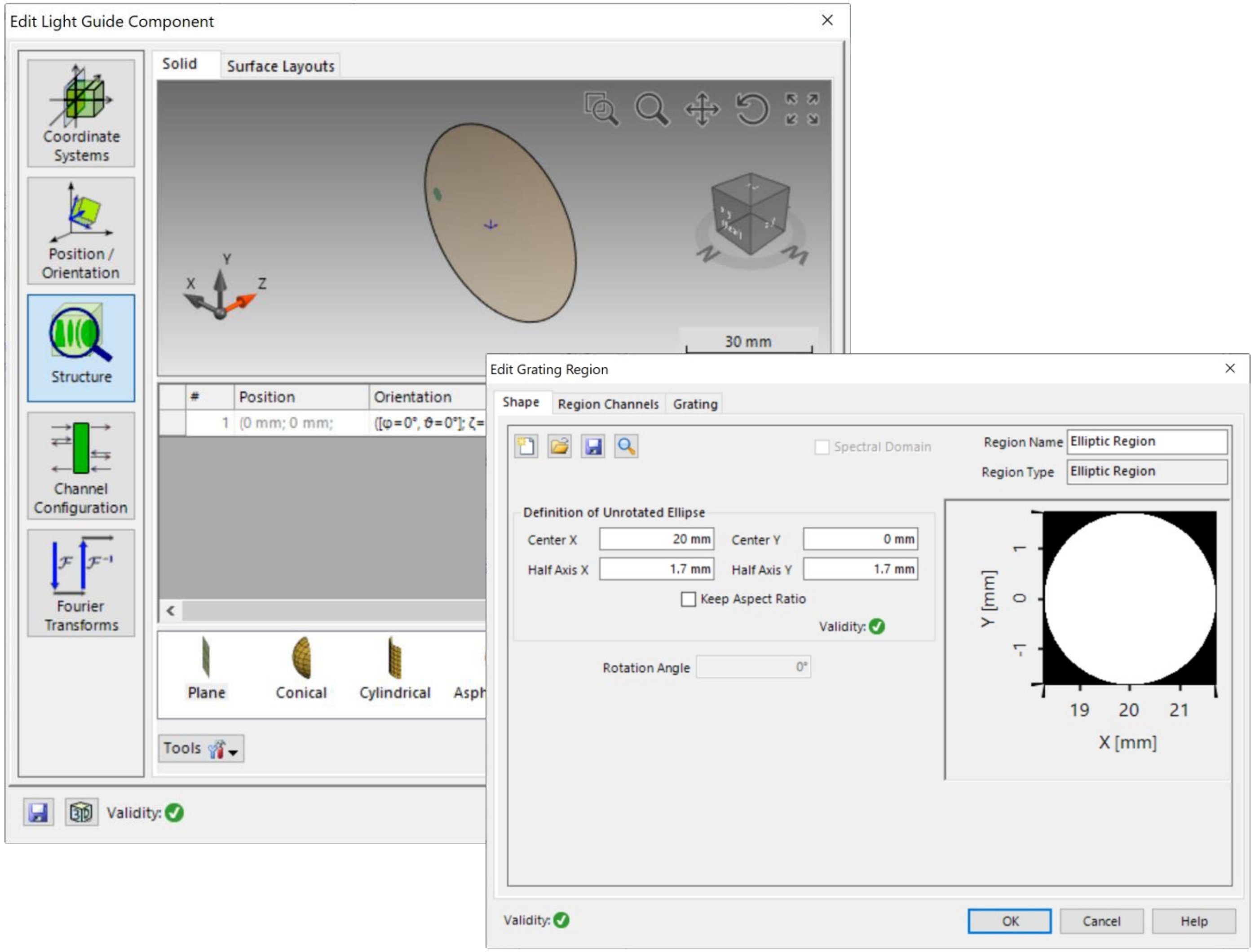
Methods	Preconditions	Accuracy	Speed	Comments
transmission function	thin element	Low	Very High	Idealized version
FMM/RCWA	-	High	Low	Rigorous model
Local Planar Interface Approximation	Surface not in focal region of beam	High	High	Local application of S matrix; LPIA; x-domain

In our case, the beam is narrow enough to not interact with the hole overall, for that reason a functional approach is sufficient.

Hole



The hole in the first mirror is modeled as an idealized transmission grating defined in a circular region with only the 0th order in transmission activated. To this order we manually assign an efficiency of 100%, in order to replicate the behavior of the hole.



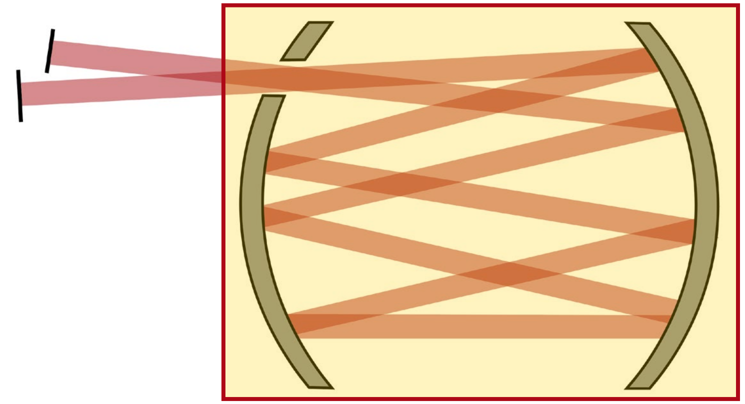
#	Position	Orientation
1	(0 mm; 0 mm;	([φ=0°, ϑ=0°]; ζ=

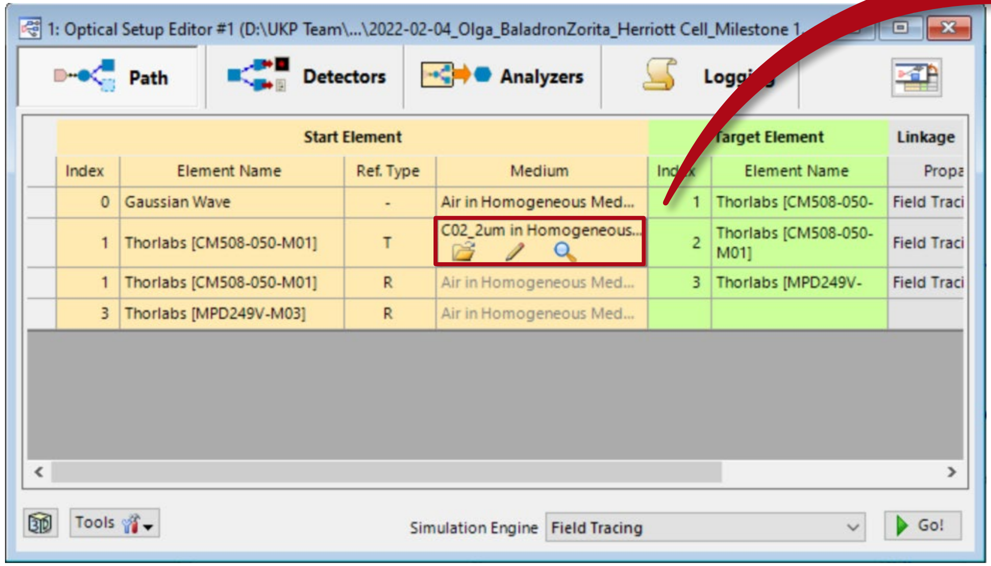
Region Name: Elliptic Region
Region Type: Elliptic Region

Definition of Unrotated Ellipse

Center X: 20 mm
Center Y: 0 mm
Half Axis X: 1.7 mm
Half Axis Y: 1.7 mm
☐ Keep Aspect Ratio
Validity: ✓
Rotation Angle: 0°
Validity: ✓

Carbon Dioxide

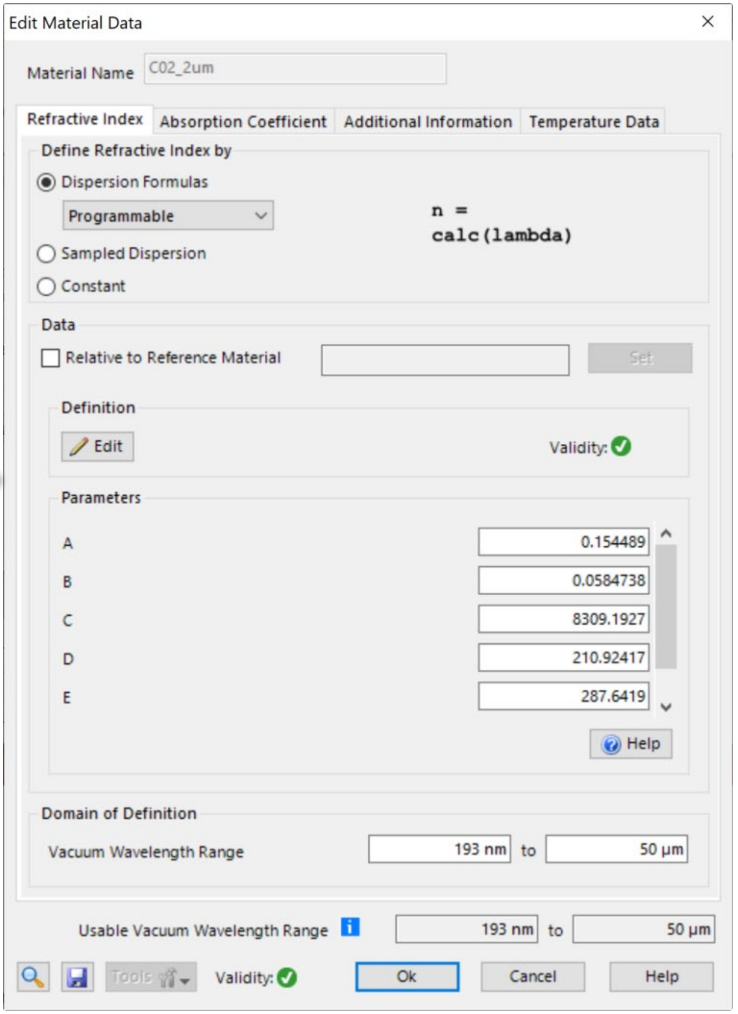




1: Optical Setup Editor #1 (D:\UKP Team\...\2022-02-04_Olga_BaladronZorita_Herriott Cell_Milestone 1

Start Element				Target Element		Linkage
Index	Element Name	Ref. Type	Medium	Index	Element Name	Propa
0	Gaussian Wave	-	Air in Homogeneous Med...	1	Thorlabs [CM508-050-	Field Traci
1	Thorlabs [CM508-050-M01]	T	C02_2um in Homogeneous...	2	Thorlabs [CM508-050-M01]	Field Traci
1	Thorlabs [CM508-050-M01]	R	Air in Homogeneous Med...	3	Thorlabs [MPD249V-	Field Traci
3	Thorlabs [MPD249V-M03]	R	Air in Homogeneous Med...			

Simulation Engine: Field Tracing



Edit Material Data

Material Name: C02_2um

Define Refractive Index by

● Dispersion Formulas

Programmable

○ Sampled Dispersion

○ Constant

```
n =
calc(lambda)
```

Data

☐ Relative to Reference Material

Definition

Validity: ✓

Parameters

A	0.154489
B	0.0584738
C	8309.1927
D	210.92417
E	287.6419

Domain of Definition

Vacuum Wavelength Range: 193 nm to 50 µm

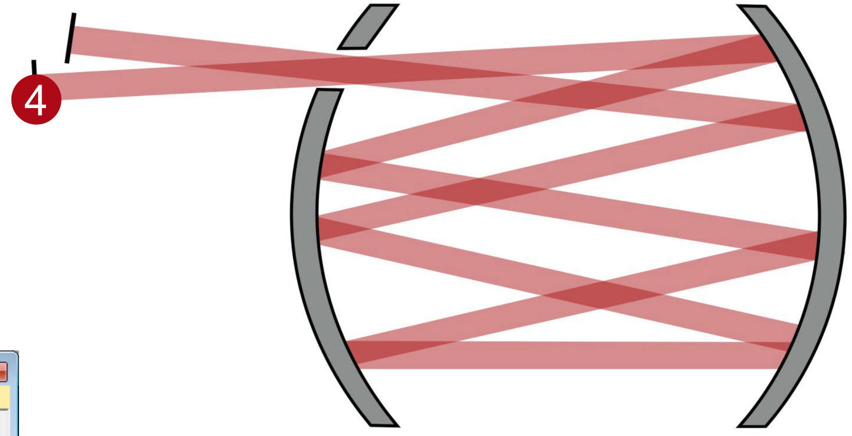
Usable Vacuum Wavelength Range: 193 nm to 50 µm

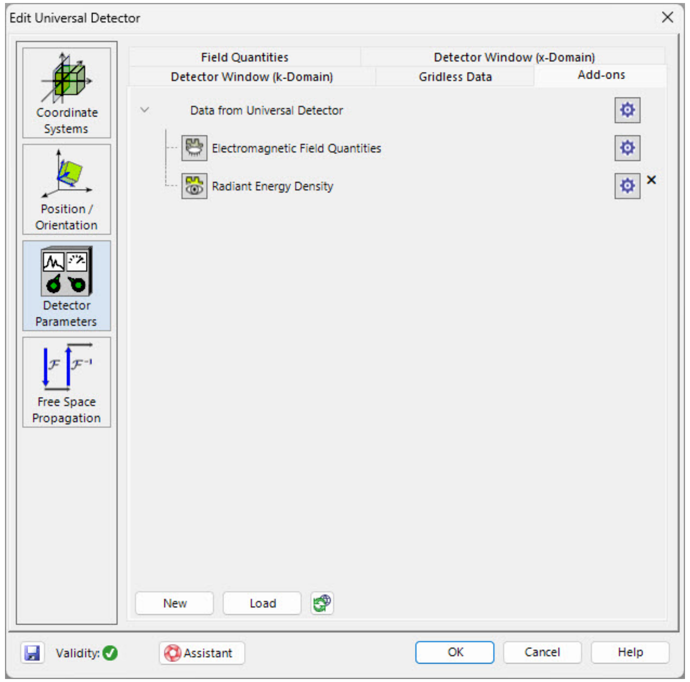
Validity: ✓

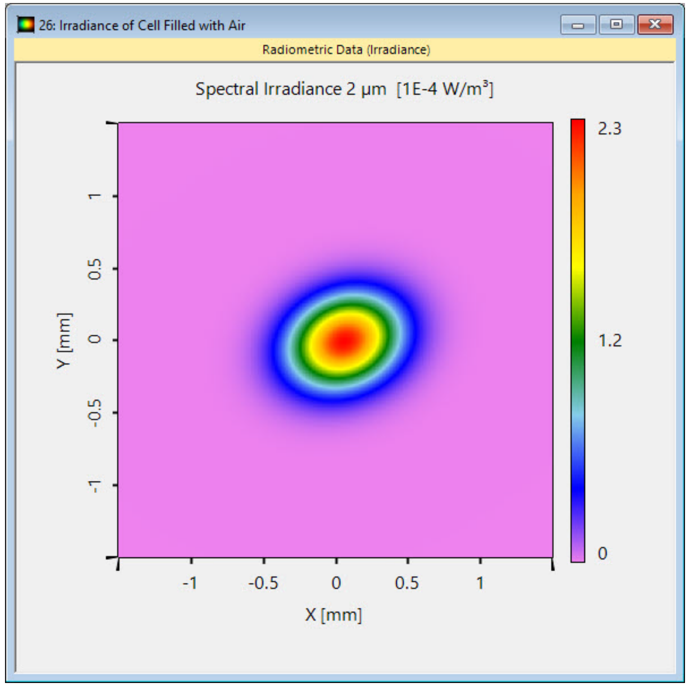
When using a material that is not available in the *Materials* Catalog, it is possible to program it using the *Programmable Material.*

Connected Modeling Techniques: Detector

① free-space propagation
② reflection at the mirrors of the cell
③ propagation through the hole
④ detector





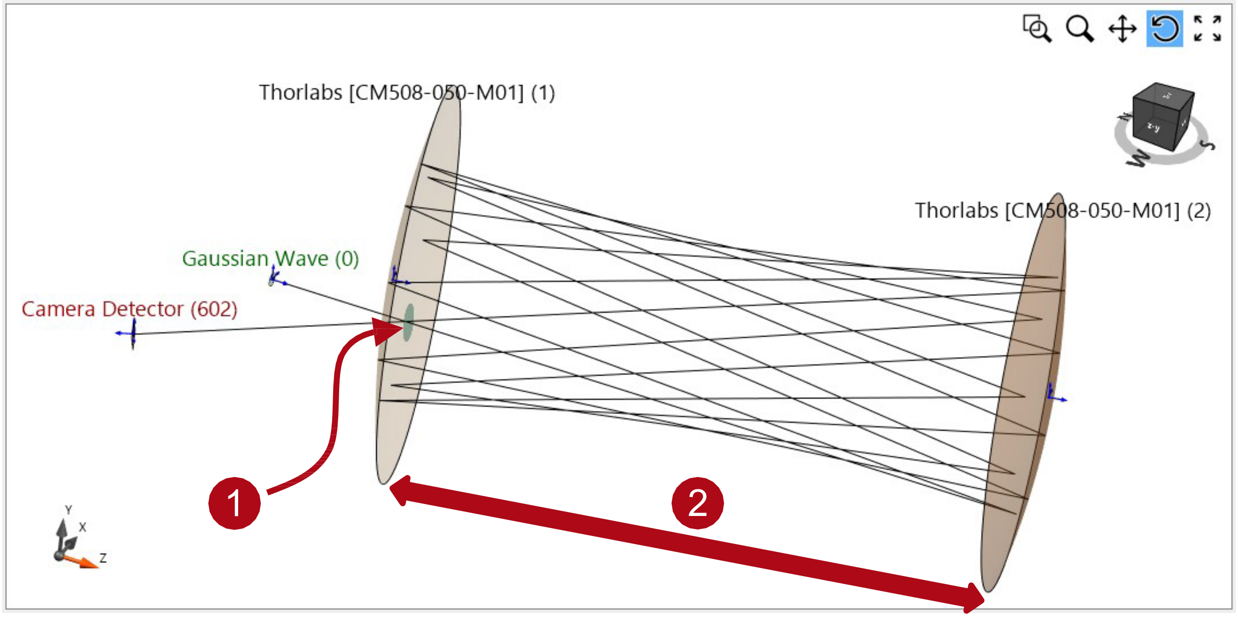


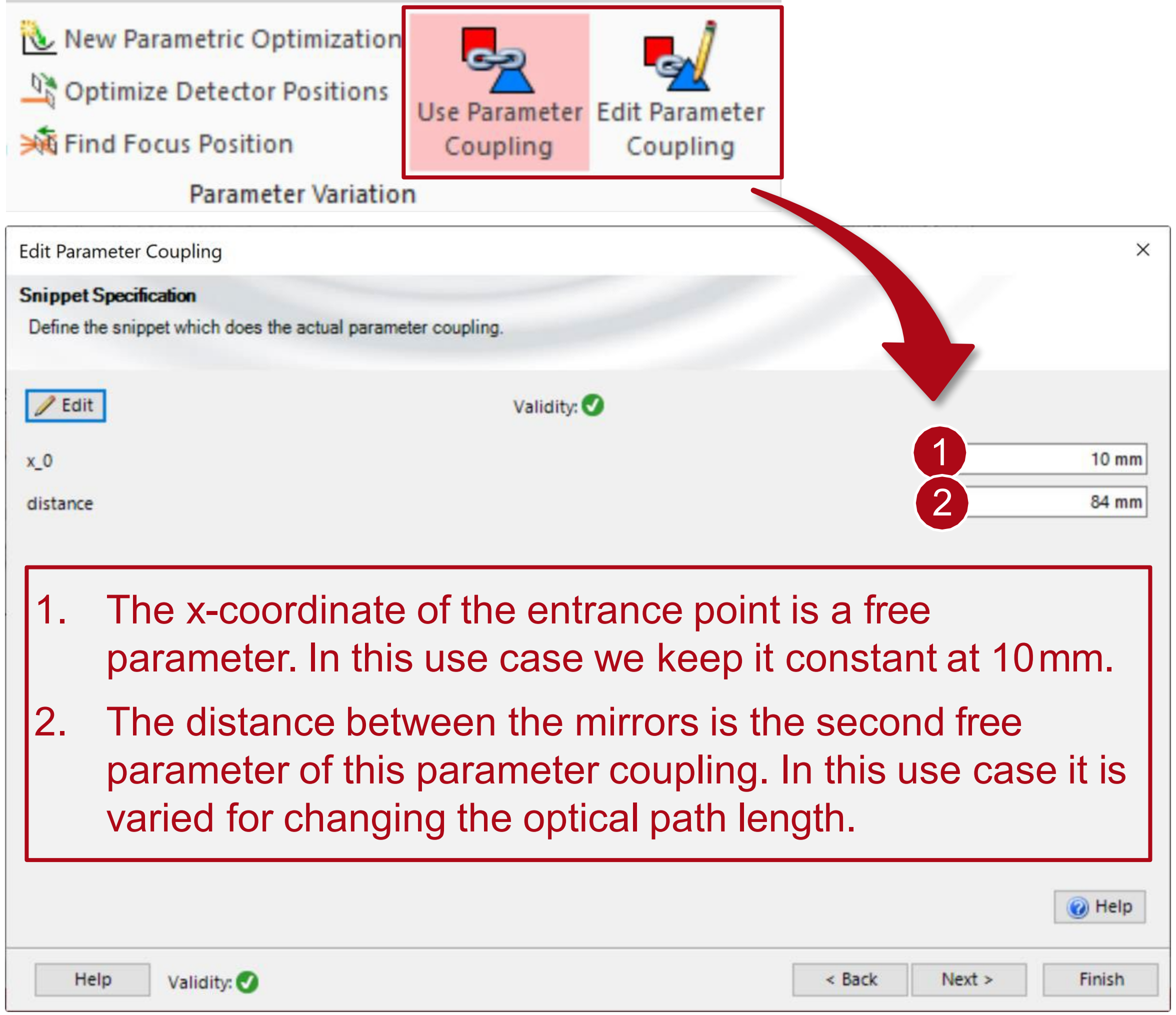
Full flexibility in detector modeling of different physical values, including e.g. the radiant energy density.

Parameter Coupling

The *Parameter Coupling* feature can be used to link parameters of the system, so that a certain relationship between them is maintained. In this case, we want to ensure a circular pattern in the distribution of the beam paths inside the Herriott cell, as a function of the x-coordinate (1) of the entrance point and the length of the cell (2).
More information about the *Parameter Coupling* under:

Coupling of Parameters in VirtualLab Fusion





Edit Parameter Coupling

Snippet Specification

Define the snippet which does the actual parameter coupling.

Validity: ✓

x_0: 10 mm

distance: 84 mm

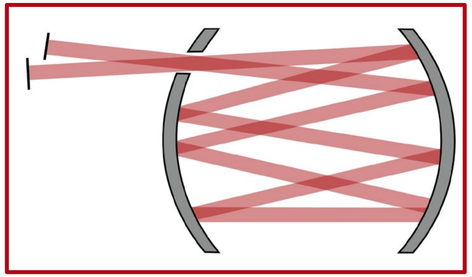
Validity: ✓

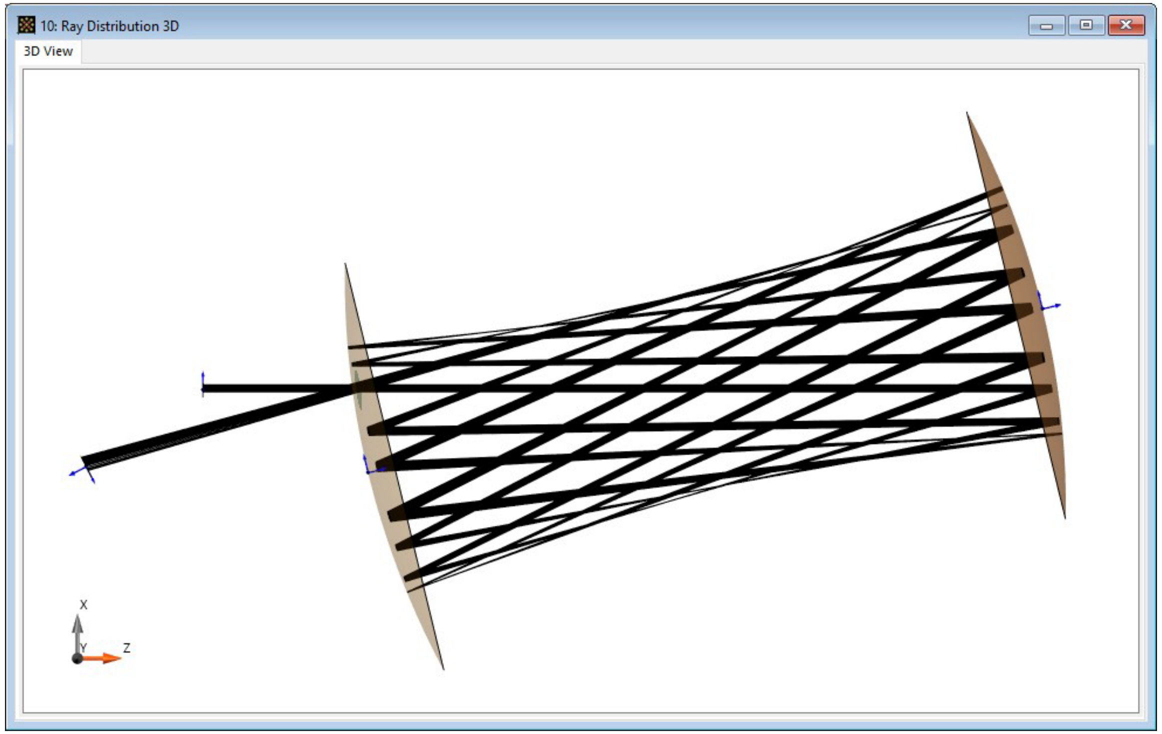
1. The x-coordinate of the entrance point is a free parameter. In this use case we keep it constant at 10 mm.
2. The distance between the mirrors is the second free parameter of this parameter coupling. In this use case it is varied for changing the optical path length.

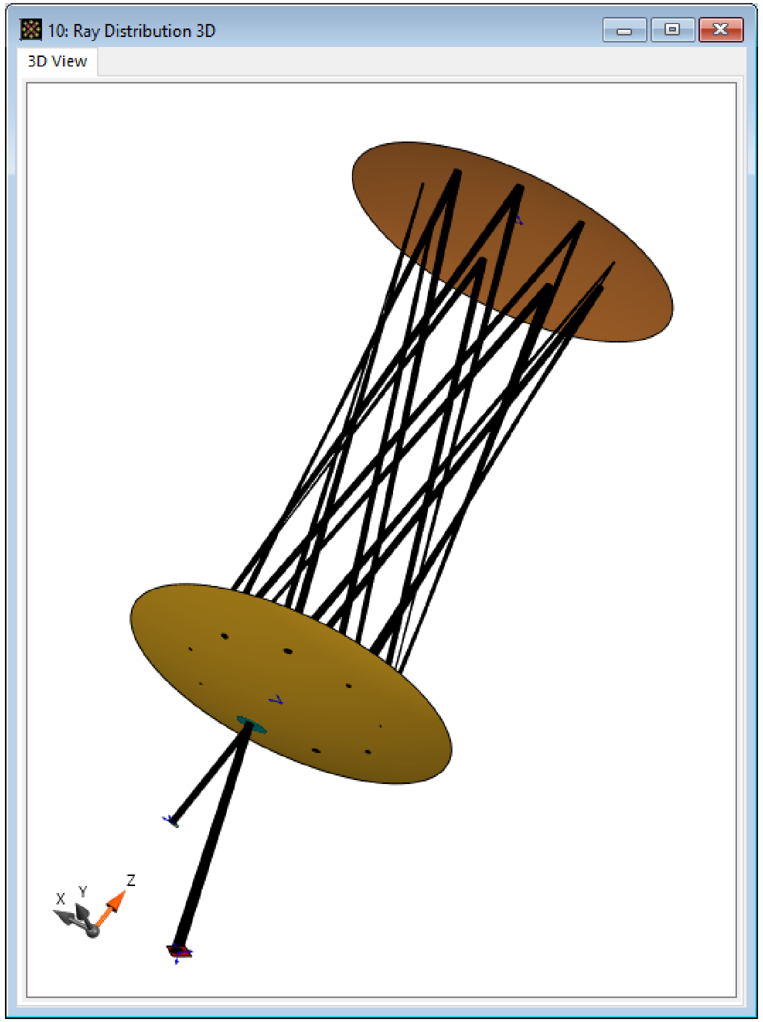
Formulas are taken from: *D. R. Herriot, H. Kogelnik, and R. Kompfner, "Off-axis paths in spherical mirror interferometers," Appl. Opt. 3, 523–526 (1964).*

Simulation Results

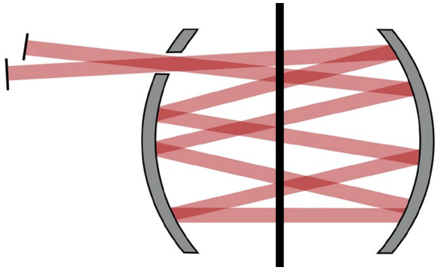
Ray Tracing Results



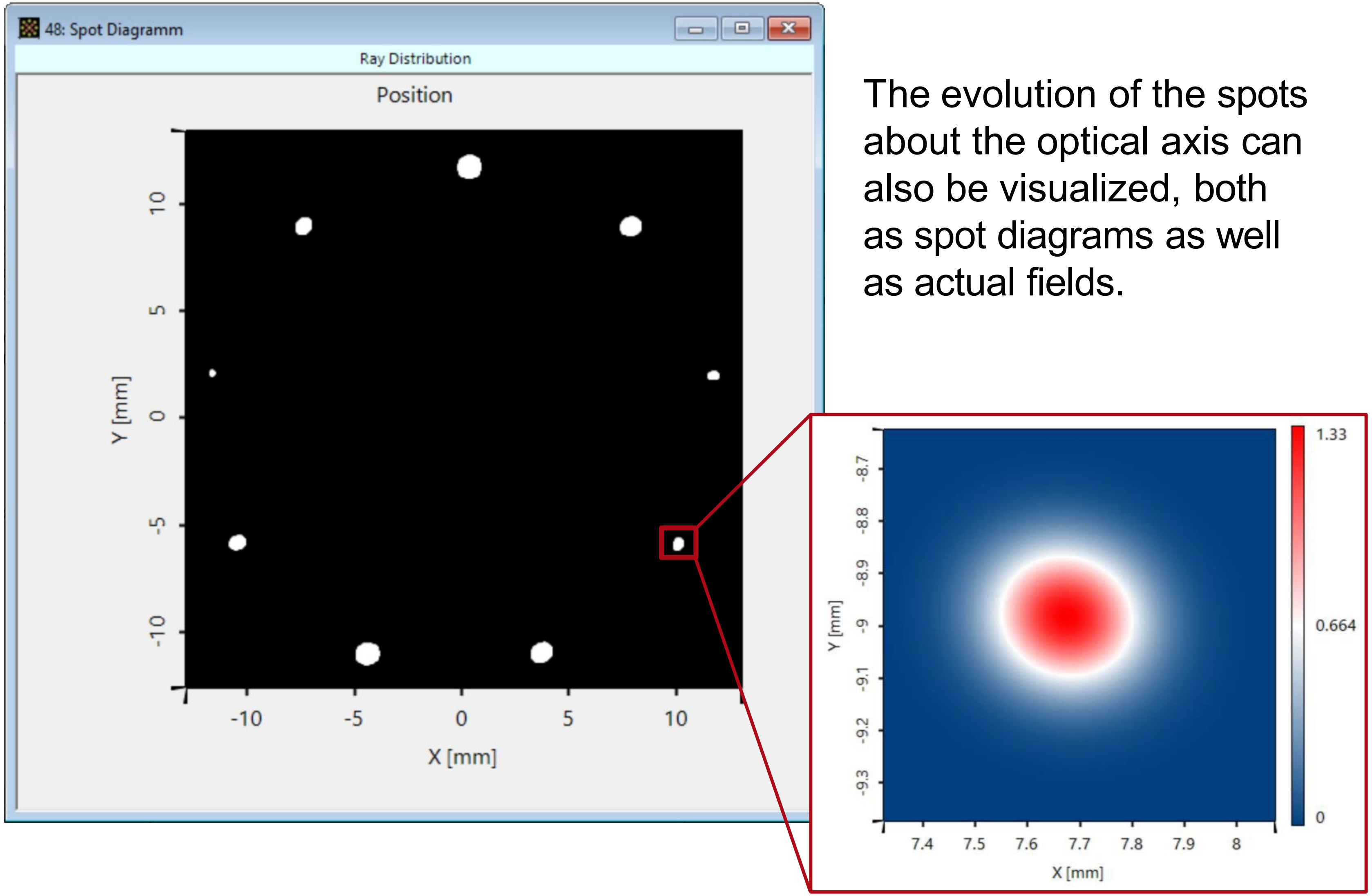




Ray & Field Tracing Results

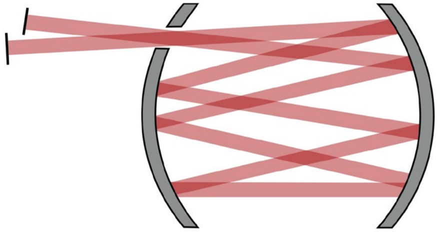


With the non-sequential approach in VirtualLab Fusion, the system will automatically determine how many revolutions the multiple-pass light path will make around the optical axis until it hits the exit hole.

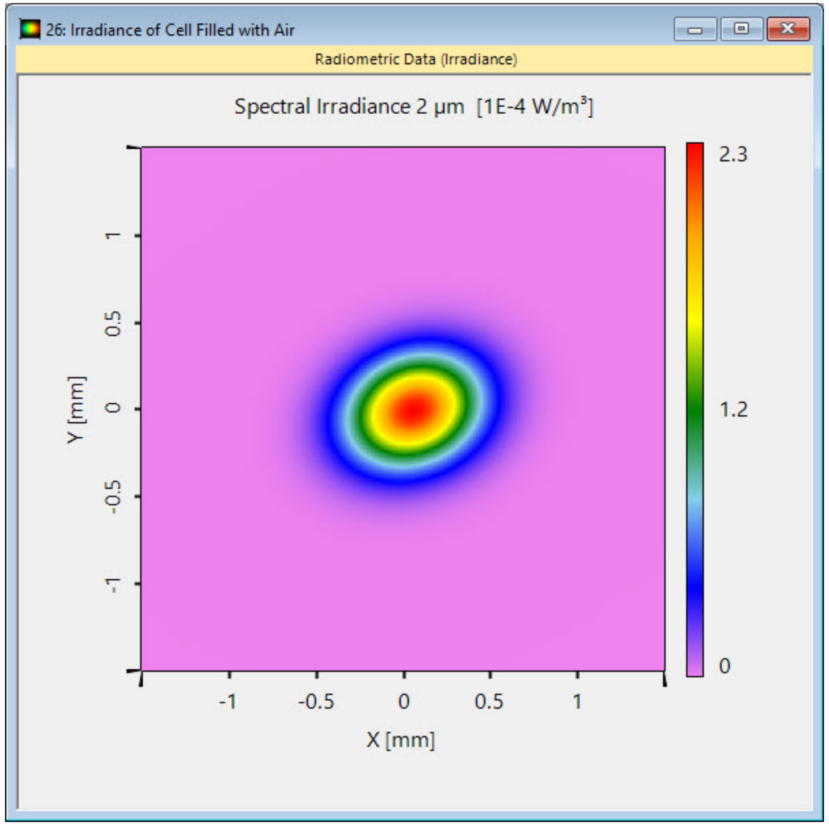


The evolution of the spots about the optical axis can also be visualized, both as spot diagrams as well as actual fields.

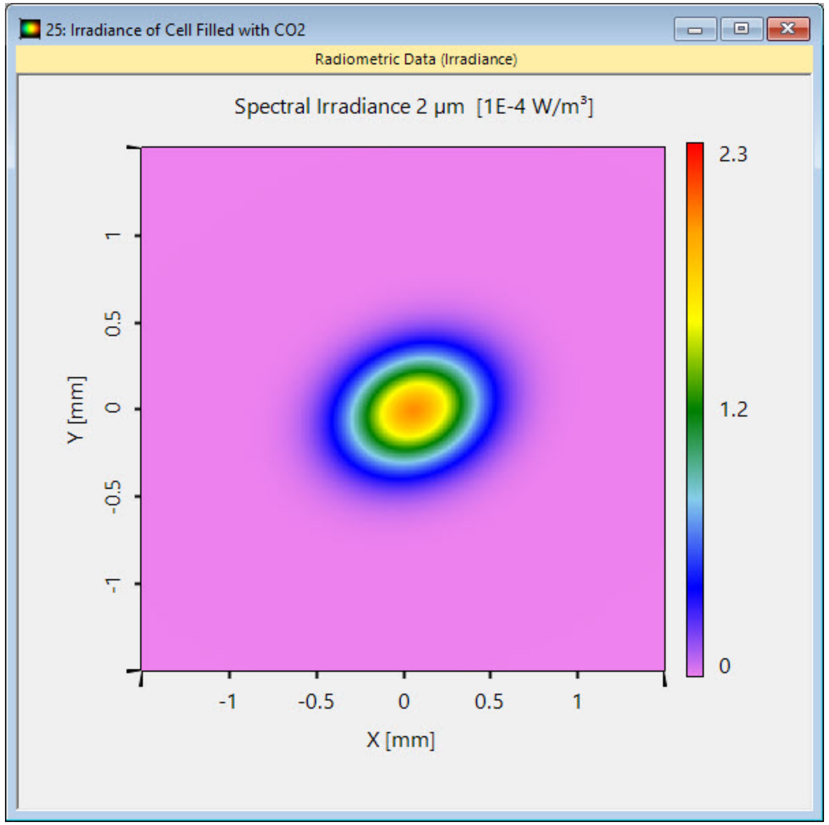
Field Tracing Results (with Mirror Distance of 84mm)



When the Herriott cell is filled with an absorptive gas (such as carbon dioxide for a beam with wavelength of 2µm) the decrease in amplitude can be measured after the resonator. Because of the low number of iterations in this design the effect is still weak, as can be observed from the figures on the right.

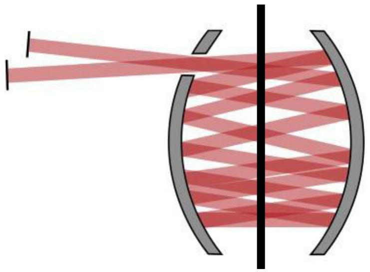


Herriott cell filled with air (reference)

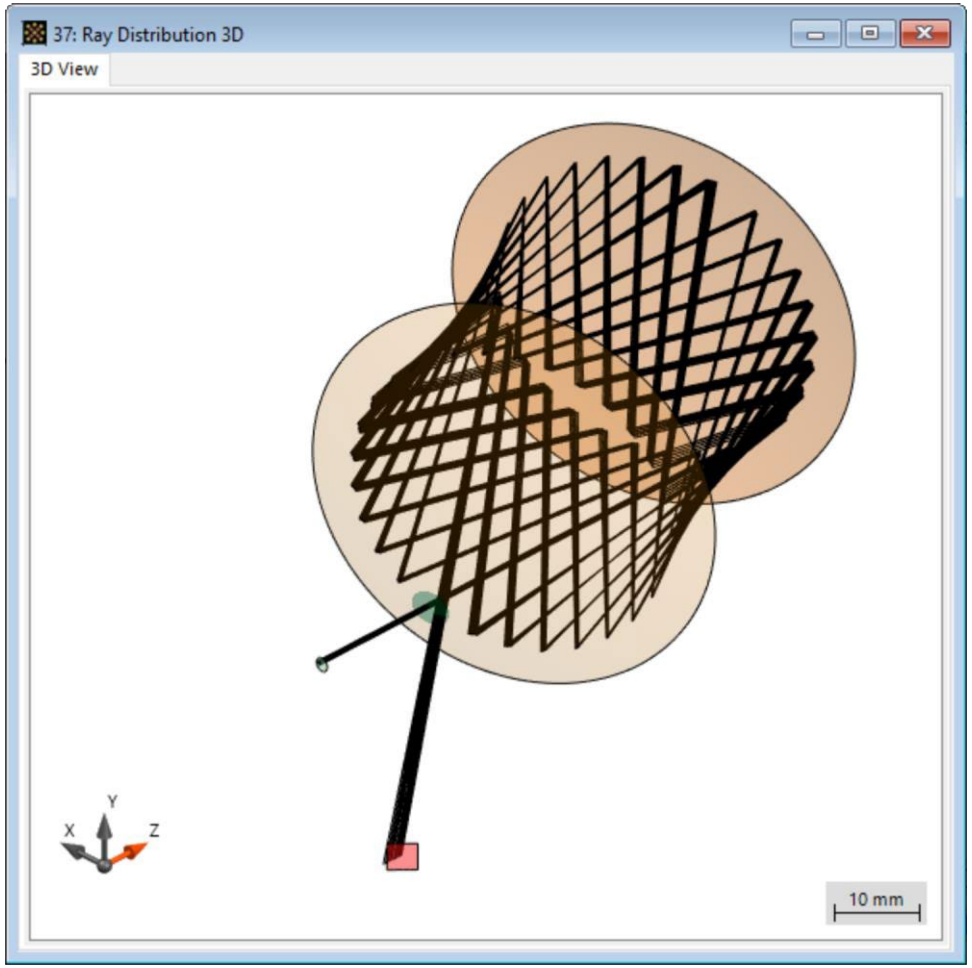


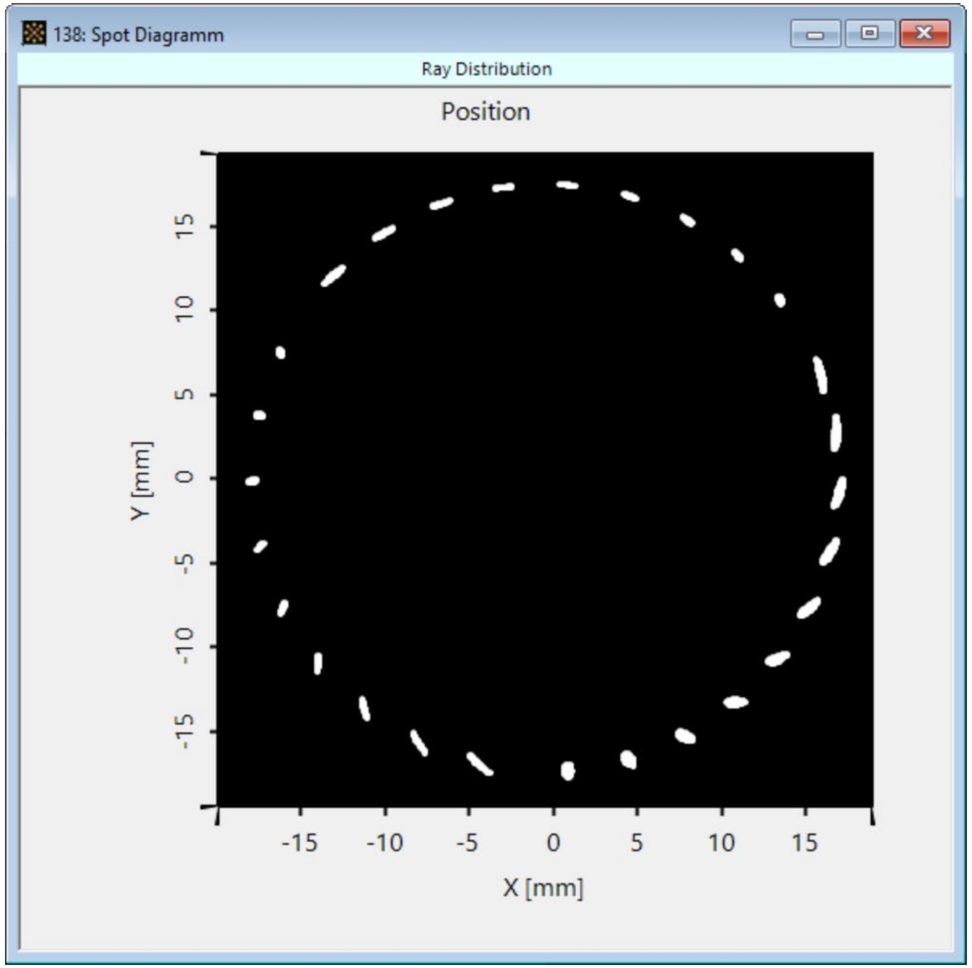
Herriott cell filled with CO_2

More Internal Reflections



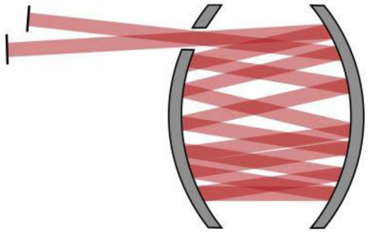
The number of iterations depends on how often the beam will make its way about the optical axis until it hits the entrance point again. This can be manipulated by adjusting either the distance between mirrors or their curvature.



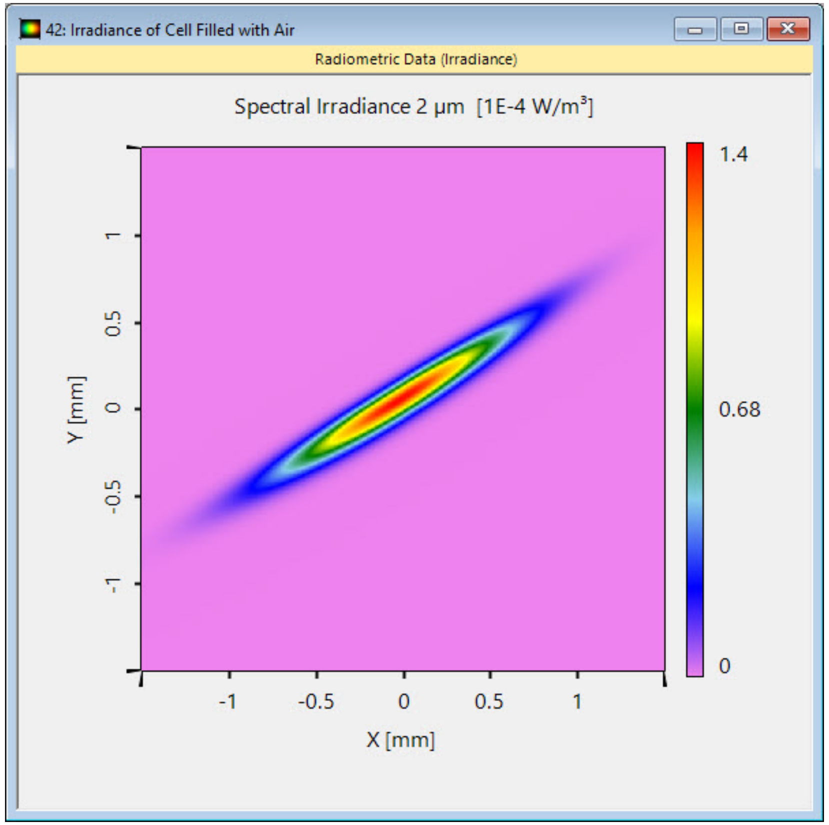


An in-depth formulation of how these parameters contribute to the number of iterations can be found in:
D. R. Herriot, H. Kogelnik, and R. Kompfner, "Off-axis paths in spherical mirror interferometers," Appl. Opt. 3, 523–526 (1964).

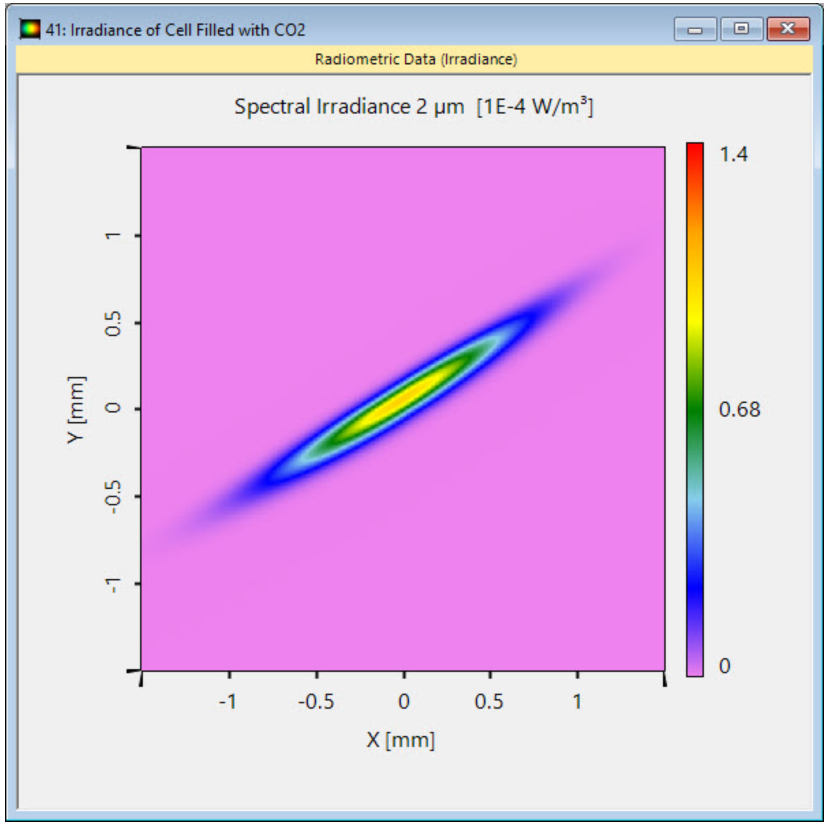
Field Tracing Results (with mirror distance of 50 mm)



A reduced resonator length leads to a stable Herriott cell with a higher number of iterations and therefore a net increase of the optical path length. This in turn leads to more absorption which can then be evaluated after the resonator.



Herriott cell filled with air (reference)



Herriott cell filled with CO_2

Document Information

title	Modeling of a Herriott Cell
document code	Misc.0094
document version	1.1
software edition	VirtualLab Fusion Basic
software version	2023.1 (Build 1.556)
category	Application Use Case
further reading	- Coupling of Parameters in VirtualLab Fusion - Examination of Sodium D Lines with Etalon