# SpecLTE: App for Simulation of Side-on Radiation Spectra from Non-uniform, Axial-symmetric LTE plasmas

## Application Help

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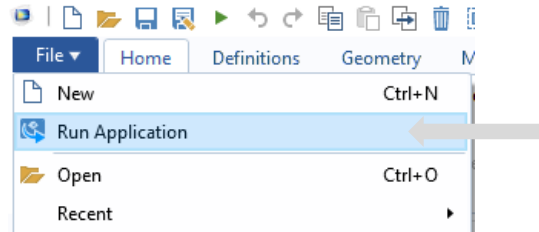School of Electrical Engineering and Computer Science, 100 44, Stockholm, Sweden

# About SpecLTE

- SpecLTE is a COMSOL application that contains a model to perform simulation of the radiation spectra emitted by a non-uniform, cylindrical plasma in Local Thermodynamic Equilibrium (LTE). The detailed information about the model is described in detail in M. Becerra et al., J. Phys. D: App Phys 52 (2019) 434003 (10pp). Any derivate work from SpecLTE should cite this reference as source.

- SpecLTE is created in COMSOL Multiphysics and can be run in versions 5.4 or superior.

- SpecLTE allows you to setup, run and visualize the spectral simulation emitted by a single specie. Data for CuI and CuII as emitter species are included in the "Example data" subfolder. The default data is for a CuII emitter with temperature and pressure profiles as in the Example data subfolder.
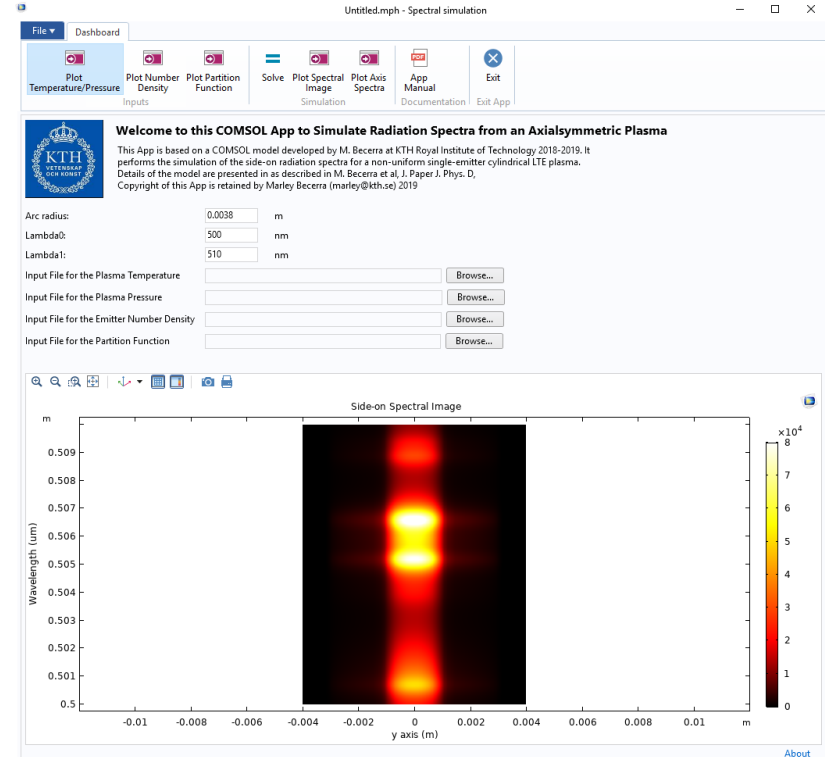
# Running SpecLTE

- Open your COMSOL Desktop environment (version 5.4 and superior) and select the Run Application to open the application

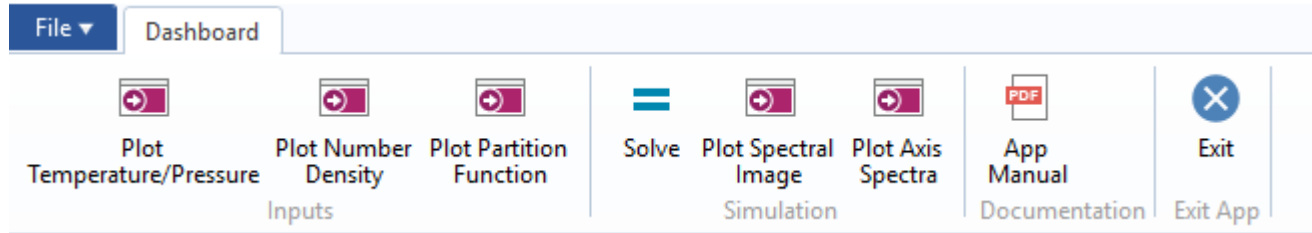After clicking, the main window of SpecLTE is launched

# SpecLTE Main Window
## Toolbar

The SpecLTE toolbar in the App allows the user to plot the main inputs of the simulation, to solve model and plot the results, to consult this App manual and to Exit the application



To run a simulation, run the icons in the toolbar from left to right. The help about how to operate the app is in the App Manual icon. To close the App, click the Exit icon.

# SpecLTE Main Window
## User Inputs

The SpecLTE user can set the radius of the plasma (used only to define the size of the spatial simulation range) and the interval within which the spectra is simulated. The spectra is simulated considering 1024 points between the defined spectral interval. He/she can also load input files containing the spatial profile for the plasma temperature and partial pressure, as well as the number density distribution of the emitter specie (as a function of temperature and partial pressure) and its corresponding partition function (as a function of temperature). SpecLTE can be set to simulate the emission from any specie granted that the correct input data is used for the emitting specie. Examples for atomic and ionic copper data as well as temperature/pressure profiles are included.

| | | |
|---|---|---|
| Arc radius: | 0.0038 | m |
| Lambda0: | 500 | nm |
| Lambda1: | 510 | nm |
| Input File for the Plasma Temperature | C:\Example data\TemperaturePlasma_Radius.txt | Browse... |
| Input File for the Plasma Pressure | C:\Example data\PressurePlasma_Radius.txt | Browse... |
| Input File for the Emitter Number Density | C:\Example data\NumberDensityCull_Pressure_Temperat | Browse... |
| Input File for the Partition Function | C:\Example data\PartitionFunctionCull_Temperature.txt | Browse... |
| Input File for Spectral Line Data | C:\Example data\AtomicSpectralDataCOMSOL_Cull.txt | Browse... |

# SpecLTE Main Window
## User Inputs: Plasma temperature & pressure

The spatial distribution of the plasma temperature and partial pressure should be given in a textfile (.txt). Click the "Browse.." button to select a proper input file:

| | | |
|---|---|---|
| Input File for the Plasma Temperature | | Browse... |
| Input File for the Plasma Partial Pressure | | Browse... |

Each file should have two, space (or tab) separated columns, with the first column defining the radial position (in m) of either the temperature (in K) or pressure profiles (in Pa). No headers should be present.

TemperaturePlasma_Radius.txt - Notepad

File  Edit  Format  View  Help
```
0 19100
4e-4 19755
8e-4 20611
1.2e-3 20790
1.6e-3 20776
2e-3 20500
2.8e-3 19305
3.3e-3 15500
3.5e-3 5000
4e-3 2000
```

PressurePlasma_Radius.txt - Notepad

File  Edit  Format  View  Help
```
0 1.012e5
3e-4 1.01e5
6e-4 1.01e5
0.9e-3 8e4
1.2e-3 2.58e4
1.8e-3 1.21e4
2.5e-3 8.6e3
3e-3 6.29e3
3.2e-3 0
4e-3 0
```

Use the [Plot Temperature/Pressure] icon in the menu to plot and crosscheck that your input is correct
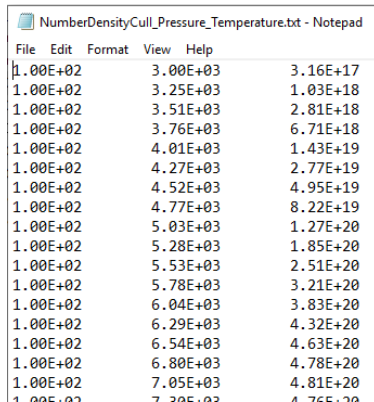
# SpecLTE Main Window
## User Inputs: Emitter Number Density

The number density of the emitting specie as a function of pressure and temperature should be given in a textfile (.txt). Click the "Browse.." button to select a proper input file:

| Input File for the Emitter Number Density | | Browse... |
| --- | --- | --- |

The file should have three, space (or tab) separated columns, with columns defining the partial pressure (in Pa), temperature (in K) and the emitter number density (in $m^{-3}$). No headers should be present.

```
NumberDensityCull_Pressure_Temperature.txt - Notepad
File  Edit  Format  View  Help
1.00E+02       3.00E+03      3.16E+17
1.00E+02       3.25E+03      1.03E+18
1.00E+02       3.51E+03      2.81E+18
1.00E+02       3.76E+03      6.71E+18
1.00E+02       4.01E+03      1.43E+19
1.00E+02       4.27E+03      2.77E+19
1.00E+02       4.52E+03      4.95E+19
1.00E+02       4.77E+03      8.22E+19
1.00E+02       5.03E+03      1.27E+20
1.00E+02       5.28E+03      1.85E+20
1.00E+02       5.53E+03      2.51E+20
1.00E+02       5.78E+03      3.21E+20
1.00E+02       6.04E+03      3.83E+20
1.00E+02       6.29E+03      4.32E+20
1.00E+02       6.54E+03      4.63E+20
1.00E+02       6.80E+03      4.78E+20
1.00E+02       7.05E+03      4.81E+20
1.00E+02       7.30E+03      4.76E+20
```

Use the [Plot Number Density] icon in the menu to plot and crosscheck that your input is correct

# SpecLTE Main Window
## User Inputs: Emitter Partition Function

The partition of the emitting specie as a function of temperature should be given in a textfile (.txt). Click the "Browse.." button to select a proper input file:

Input File for the Partition Function [                                    ] Browse...

The file should have two, space (or tab) separated columns, with the columns defining the temperature (in K) and the partition function. No headers should be present.

PartitionFunctionCull_Temperature.txt - Notepad

File  Edit  Format  View  Help

```
1000  1
2000  1
3000  1.0003
4000  1.0049
5000  1.0253
7000  1.1672
10000  1.6979
13000  2.5373
16000  3.5985
19000  4.8698
21000  5.8482
23000  6.9417
25000  8.1533
30000  11.657
```

Use the [Plot Partition Function] icon in the menu to plot and crosscheck that your input is correct

# SpecLTE Main Window
## User Inputs: Spectral Line Data

The spectral data of each of the lines considered for the emiting specie should be given in a textfile (.txt). Click the "Browse.." button to select a proper input file:

| Input File for Spectral Line Data | | Browse... |
|---|---|---|

The file should have three, space (or tab) separated columns specifying the parameter name, value and description of the spectral data for each line. For this, the central wavelength (in m), FWHM, upper energy level (in eV), the term h*c*gA/(4*pi*lambdaC), the Lorentz profile equation and the emission coefficient are sequencially defined for each line considered for the emitting specie.

Since this file needs to be compatible as a COMSOL input file and many lines may be considered, a Matlab file called CreateSpectralLineData_COMSOLVariableInputFile_APP.m has been included in the installation to automate the generation of this file.

# SpecLTE Main Window
## User Inputs: Spectral Line Data (cont)

The compiling Matlab file uses as input a datafile (.dat) with five tab separated columns for the central wavelenght (in nm), transition strength gA (in $s^{-1}$), lower energy level (in eV), upper energy level (in eV) and FWHM (in nm) of each considered line. The first four columns can be obtained from the NIST spectral line database (https://physics.nist.gov/PhysRefData/ASD/lines_form.html) as shown in the right image. The FWHM should be defined based on the instrumental broadening or estimated from measurements (as in the reference paper).

Notice that the parameters in the NIST database gives units different to those required by the App.

# SpecLTE Maintenance

This is the beta version of SpecLTE. It will be maintained by M. Becerra at KTH Royal Institute of Technology. For feedback and future cooperation in research please contact

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