CRYSTAL GROWTH SIMULATION TOOL MANUAL

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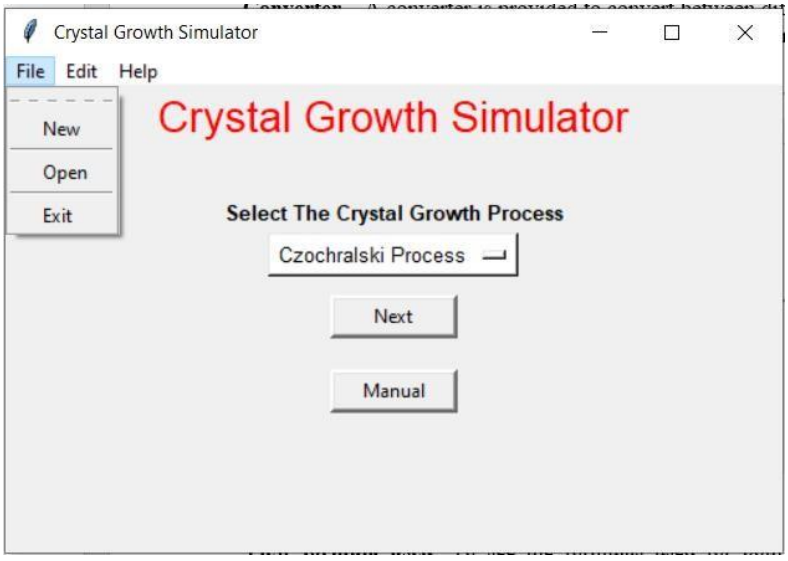
1. Tool Overview

Open the application by clicking on the .exe. Below is the interface of crystal growth simulator app upon opening. This app can be used for both Czochralski and Float zone processes.

1.1 Menu

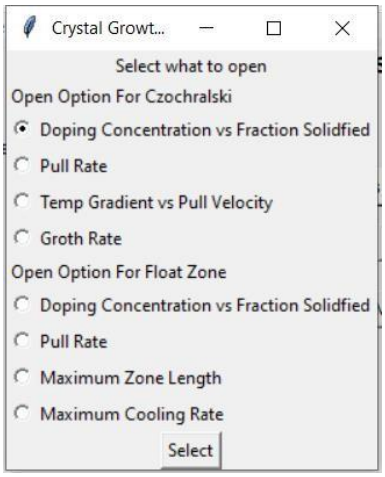
At the top there are 3 menus - **File, Edit, Help**

Menu File has the following options:



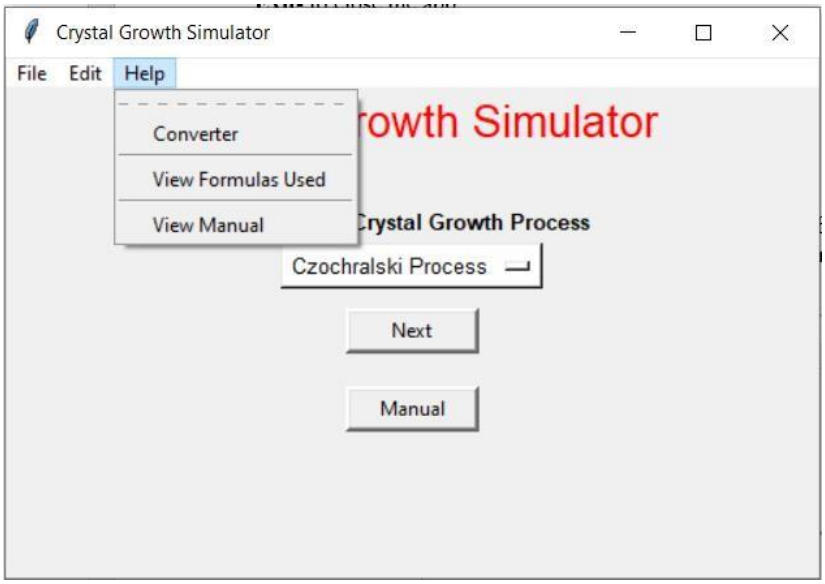
New - For opening fresh window or in case if some bugs appear.

Open – The tool provides an option of saving the data. We can open the saved data for viewing any previous work (Note: The file name and format should not be changed after saving).

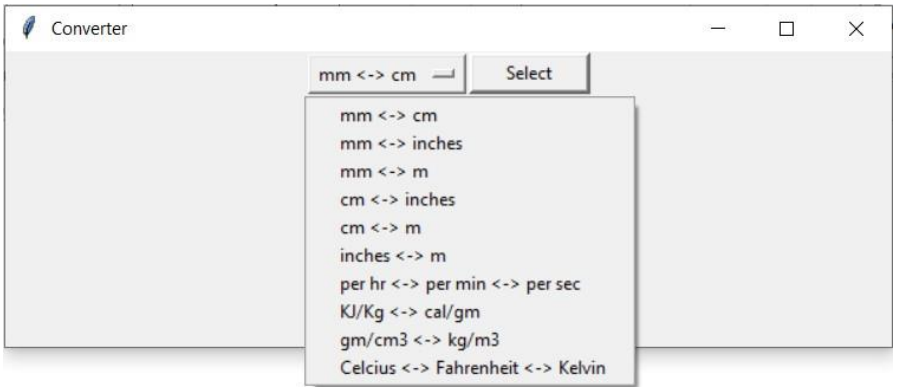


Exit- to close the app.

Help menu has following options:



Converter – A converter is provided to convert between different set of units which are used in the tool. For instance, the pull rate requires the diameter to be in inches. If one needs to convert from cm or m to inches, they can use converter.



View formula used -To see the formulas used for both the processes in pdf format or additionally the formulas are also available in the manual.

View manual -To see the manual in pdf format.

1.2 Process Simulation

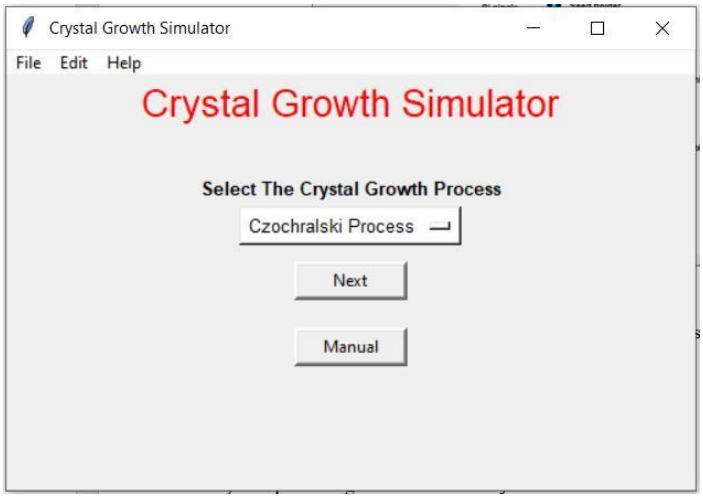
There are two crystal growth processes for which simulation is done,

1) Czochralski process
2) Float Zone process

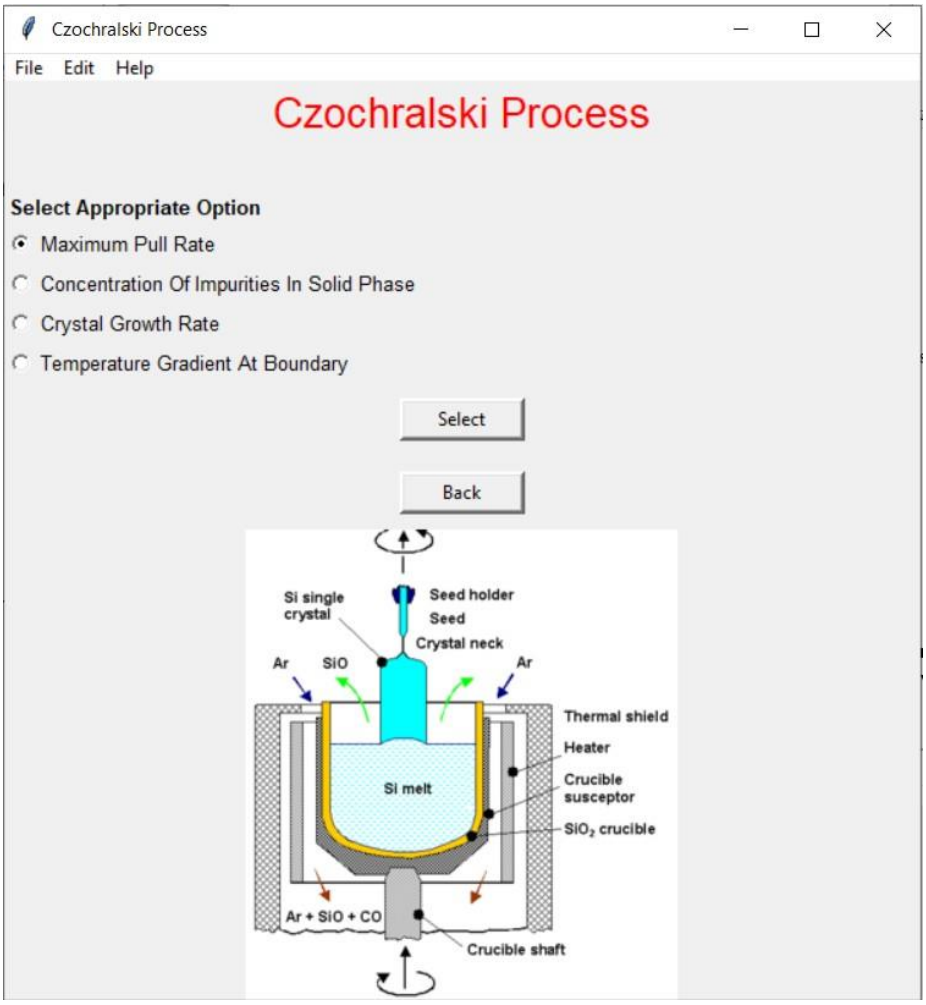
1.2.1 Czochralski Process

From the first window, select the **Czochralski process option** under select the crystal growth process

Then click on next button.



Then following window appears,



Under Czochralski Process, we can do following simulations,

1) Maximum pull rate

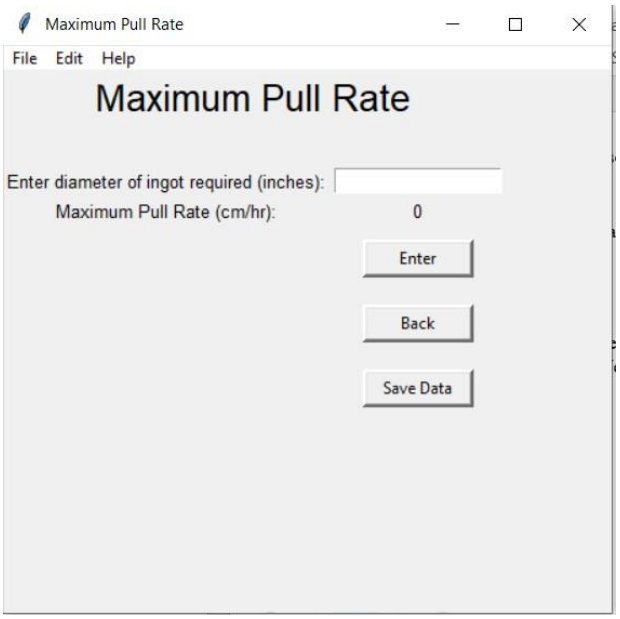
2) Concentration of impurities in solid phase

3) Crystal growth rate

4) Temperature gradient at boundary

Maximum Pull Rate

Let us choose first option i.e. if we want to find out **maximum pull rate**, click the maximum pull rate option and then select. We get the following window,



After putting appropriate values for example diameter as 12 inches then clicking on enter, we get maximum pull rate equal to 16.704 cm/hr.

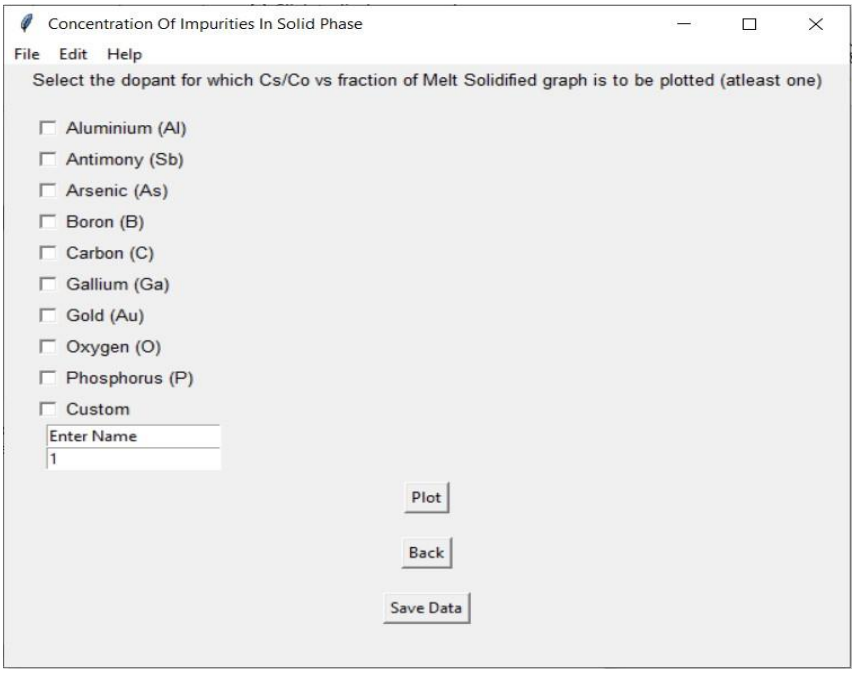
We can save our data in form of excel sheet by clicking on save data option. For each set of data entered, only those data are saved after which save data option has been pressed. For instance, if we want to save 12 inches as well as new data, say 6 inches, we have two press save data option after each time of calculation. This gives us the option to save only those data in which we are interested. The csv file will be in the same folder as the .exe.

A	B
Diameter of Ingot Required (inches)	Maximum Pull Rate (cm/hr)
12	16.70406461
6	23.62311471

We can go back to previous window any time by clicking on back option.

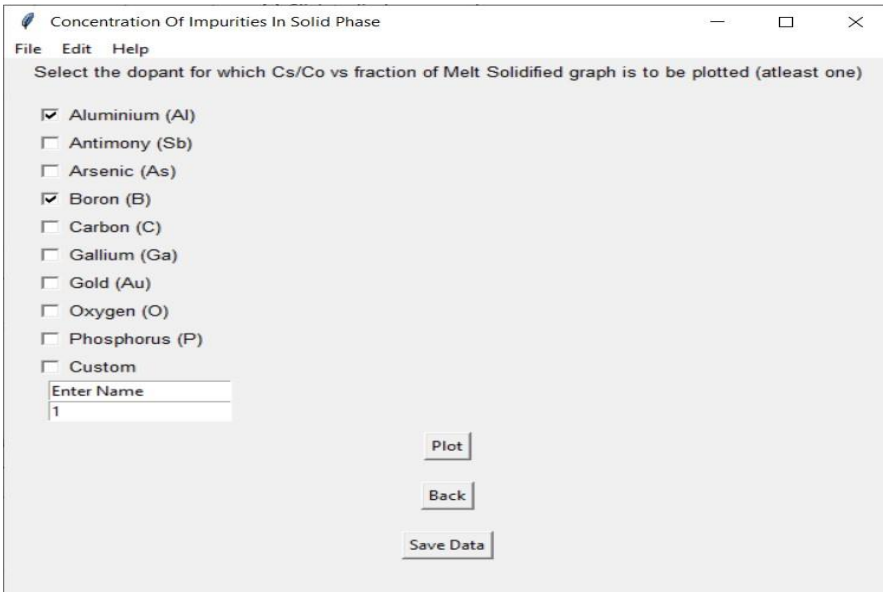
Concentration of Impurities in Solid Phase

For the second option to plot the **concentration of impurities in solid phase vs fraction solidified** waveform, click on that option and then press select. We get the following window,

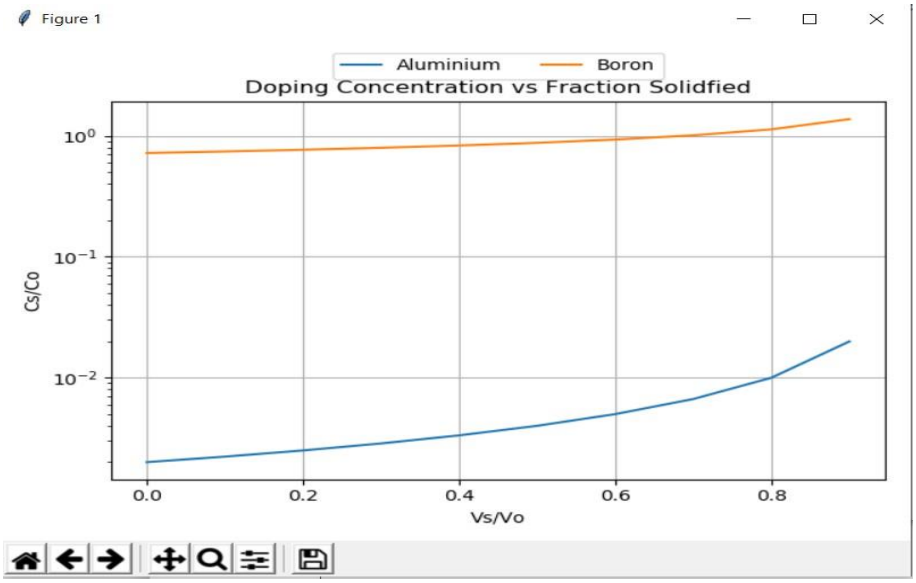


Select atleast one dopant to be plotted. We also have provided an option to enter any custom dopants which are not in the list. For this click on custom option and write its name in enter name option and write its k value that is segregation value. Default name and value is set to Enter name and 1 respectively.

Take a case for Aluminium and Boron. Select Aluminium and Boron using the checkboxes and click plot.



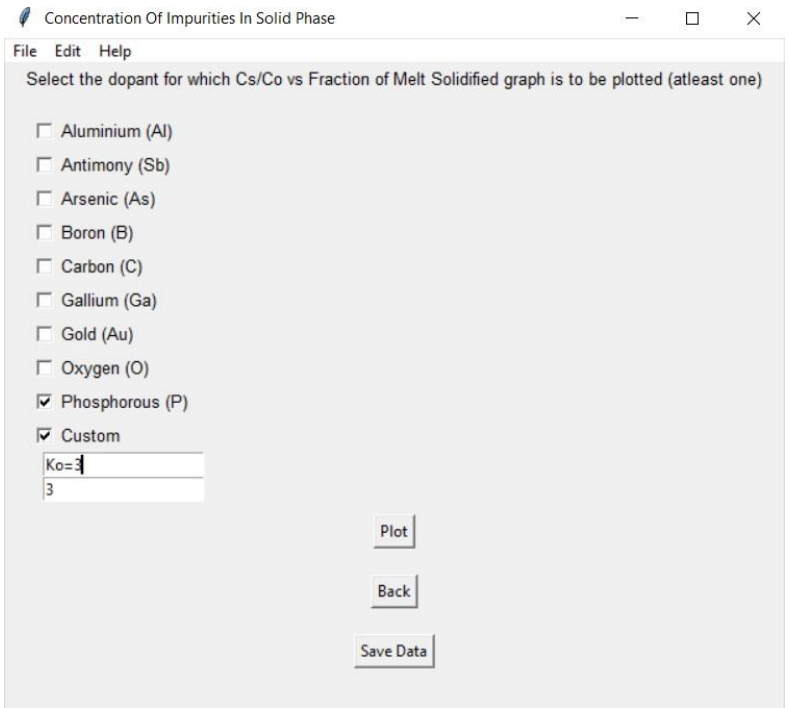
The following plot is opened,



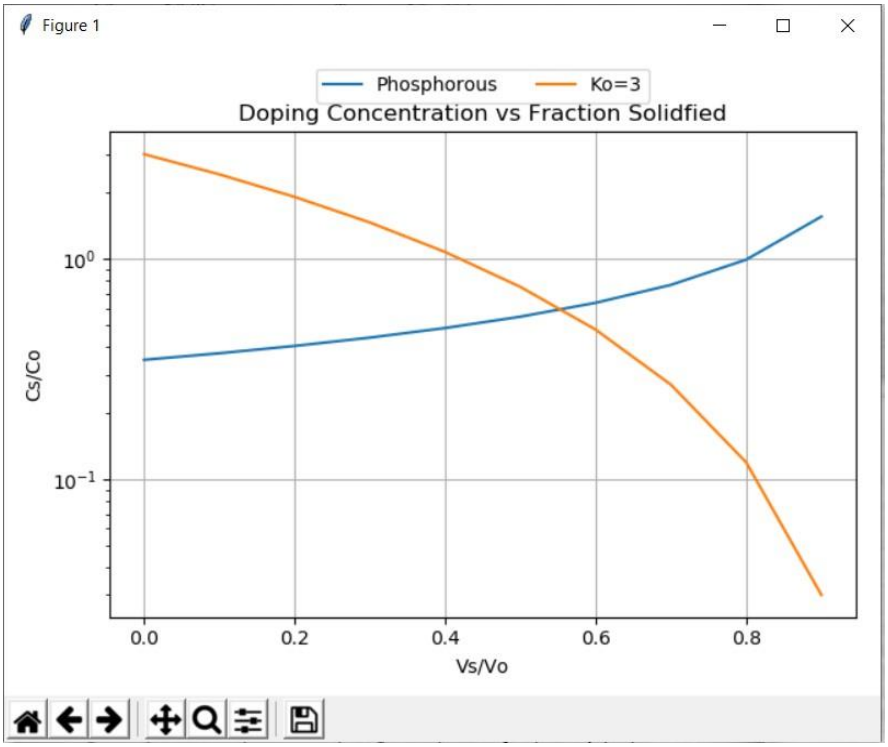
To save the set of data used for plotting, click save data. (Note: Only those data which are plotted will be saved).

A	B	C	D	E	F	G	H	I	J	K
Fraction Solidfied-->	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Aluminium (Al)	0.002	0.002222	0.002499	0.002855	0.00333	0.003994	0.004991	0.006651	0.009968	0.019908
Boron (B)	0.72	0.741557	0.766421	0.795619	0.830711	0.87422	0.930584	1.008645	1.129911	1.371932

For custom dopant, you can just click on the checkbox next to custom. Take a case for Phosphorous and custom dopant with ko=3.

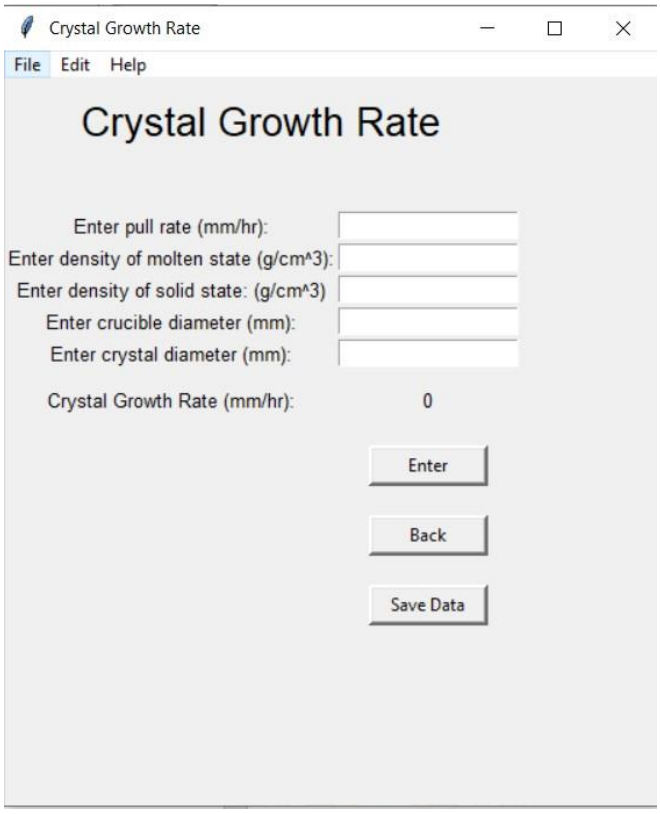


The following plot is obtained,

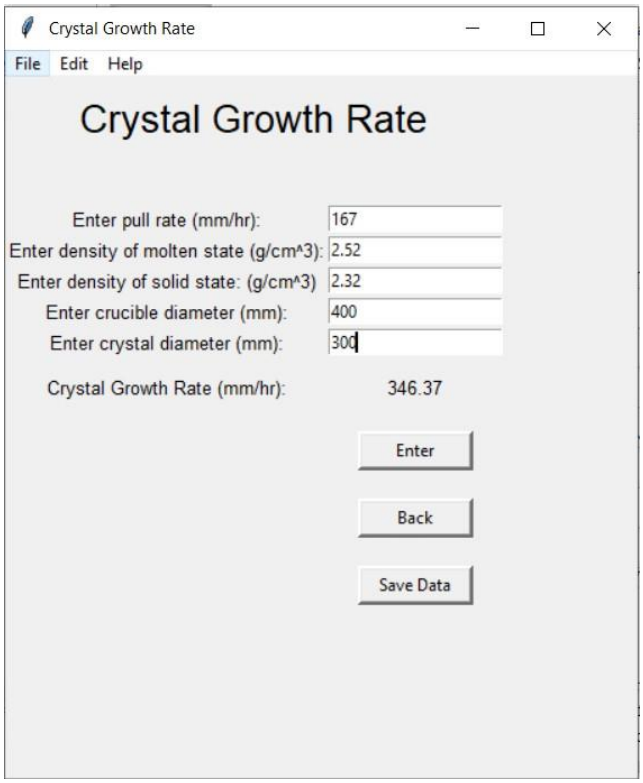


Crystal Growth Rate

To find out **crystal growth rate**, click on crystal growth rate option and then press select. Following window appears,



Let’s enter few details as follows, and press enter to calculate the crystal growth.

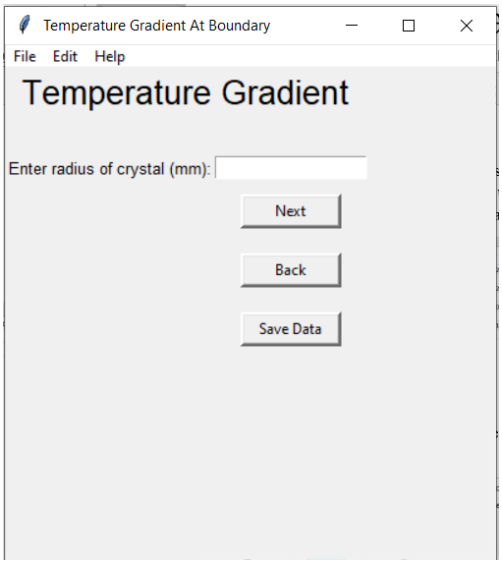


Save the data into a csv format by pressing save data.

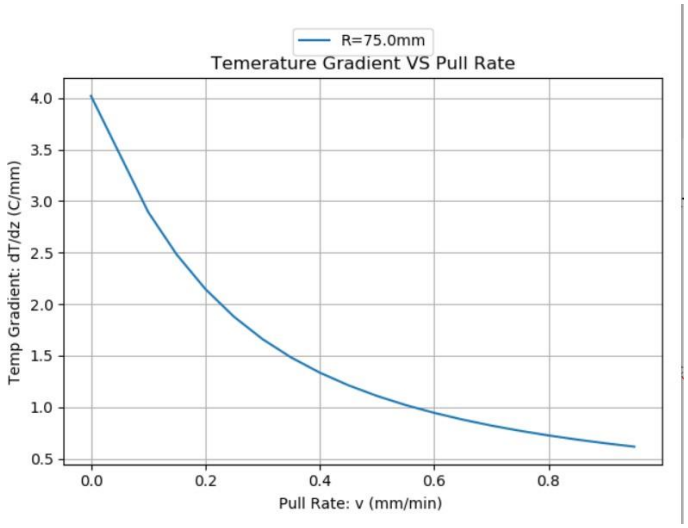
A	B	C	D	E	F
Pull Rate (mm/hr)	Density of Molten State (g/cm^3	Density of Solid State (g/cm^3)	Crucible Diameter (mm)	Crystal Diameter (mm)	Crystal Growth Rate (mm/hr)
167	2.52	2.32	400	300	346.3703704

Temperature Gradient at Boundary

To find out **temperature gradient at boundary**- click on that option then select.



Enter the radius of the crystal, for instance consider, radius of 75 mm. Press next to plot the graph. Following graph is plotted,



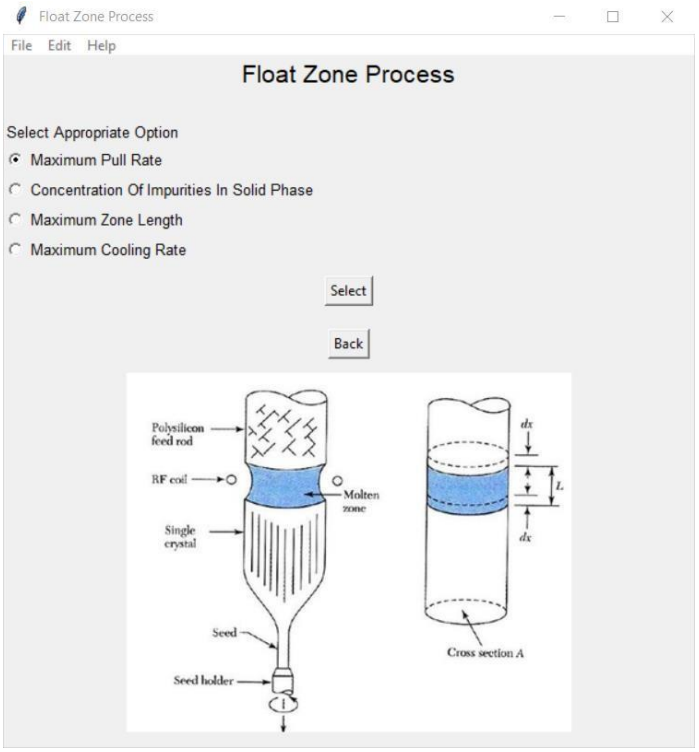
To save data in form of csv for future reference, click on save data option. All data will get saved in form of csv. Let us enter few more data options, say, 75, 200, 350.50, 175.9. We get the following data after saving into csv.

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
Pull Rate (mm/min) -->	0	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95
Temp Gradient (C/mm) for R = 75.0	4.020179	2.893837	2.480069	2.146662	1.878032	1.660409	1.482556	1.335688	1.213083	1.109633	1.021454	0.945576	0.879712	0.822082	0.771287	0.726216	0.685982	0.649864	0.617276
Temp Gradient (C/mm) for R = 75.0	4.020179	2.893837	2.480069	2.146662	1.878032	1.660409	1.482556	1.335688	1.213083	1.109633	1.021454	0.945576	0.879712	0.822082	0.771287	0.726216	0.685982	0.649864	0.617276
Temp Gradient (C/mm) for R = 350.5	1.859653	0.949844	0.726118	0.580039	0.47982	0.407771	0.353876	0.312219	0.279144	0.25229	0.230078	0.211415	0.195522	0.181831	0.169916	0.159457	0.150202	0.141957	0.134566
Temp Gradient (C/mm) for R = 175.9	2.625083	1.604297	1.292979	1.068305	0.903063	0.778498	0.682216	0.606054	0.544558	0.494004	0.451792	0.416063	0.385461	0.358974	0.335839	0.315466	0.297393	0.281257	0.266764

1.2.2 Float Zone process

From the first window, select the **Float Zone Process option** under select the crystal growth process.

Select the process and click next, the following window appears.



Under Float Zone Process, we can do following simulations,

1) Maximum pull rate

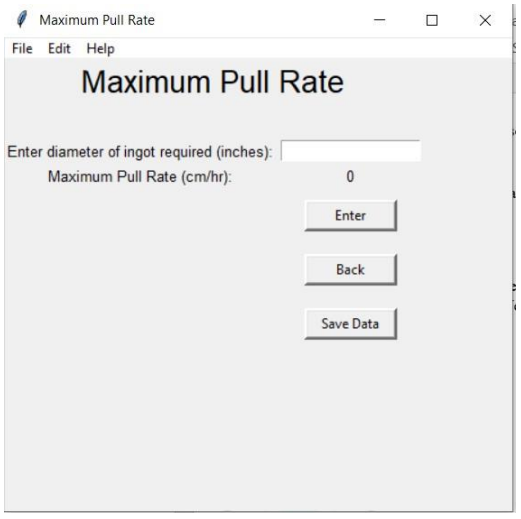
2) Concentration of impurities in solid phase

3) Maximum Zone Length

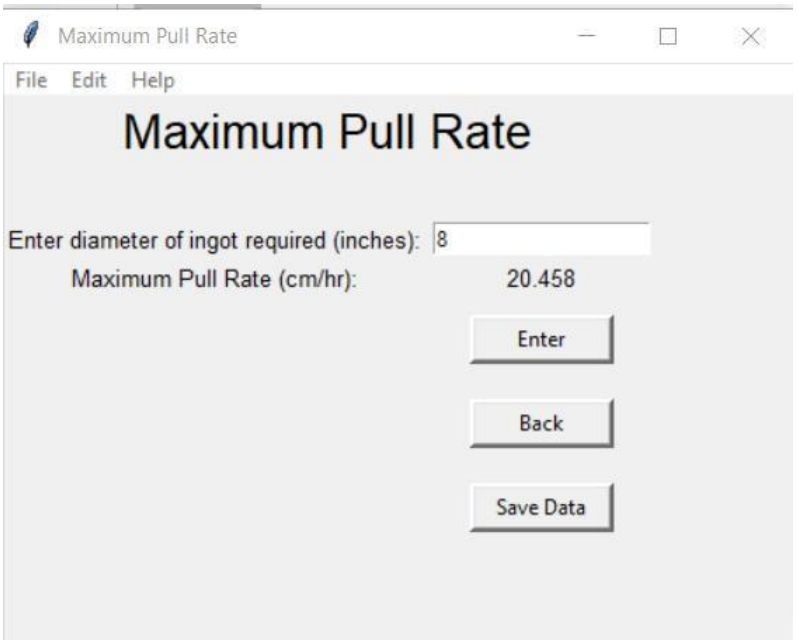
4) Maximum Cooling Rate

Maximum Pull Rate

Let us choose first option i.e. if we want to find out **maximum pull rate**, click the maximum pull rate option and then select. We get the following window,



After putting appropriate values for example diameter as 8 inches then clicking on enter, we get maximum pull rate equal to 20.458 cm/hr.



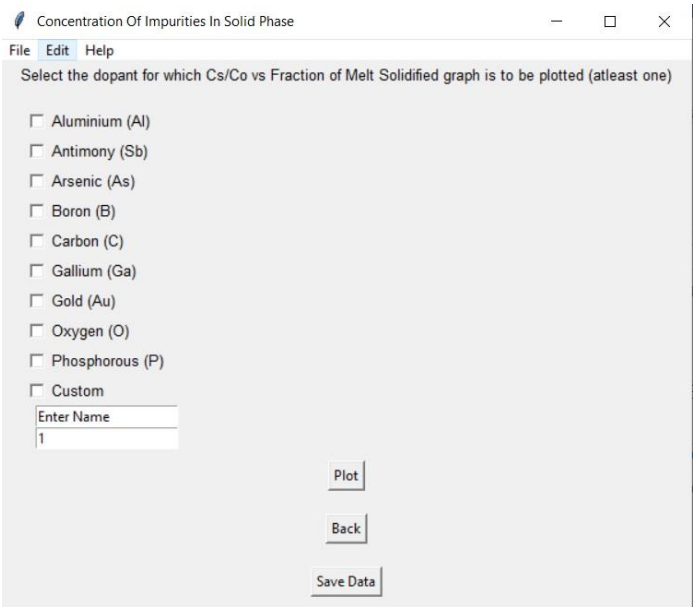
We can save our data in form of excel sheet by clicking on save data option. For each set of data entered, only those data are saved after which save data option has been pressed. For instance, if we want to save 8 inches as well as new data, say 5 inches, we have two press save data option after each time of calculation. This gives us the option to save only those data in which we are interested. The csv file will be in the same folder as the .exe.

A	B	C	D
Diameter of Ingot Required (inches)	Maximum Pull Rate (cm/hr)		
8	20.45822		
5	25.87783		

We can go back to previous window any time by clicking on back option.

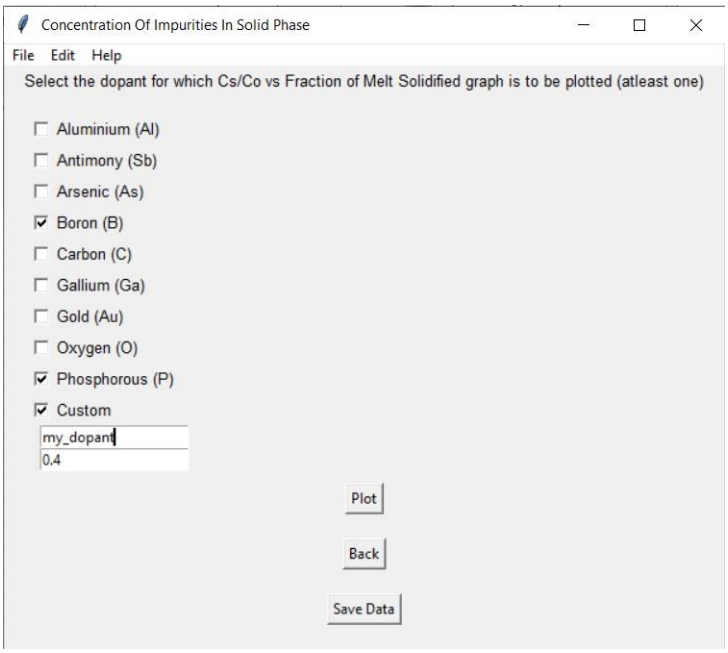
Concentration of impurities in solid phase

For the second option to plot the **concentration of impurities in solid phase vs fraction solidified** waveform, click on that option and then press select. We get the following window,

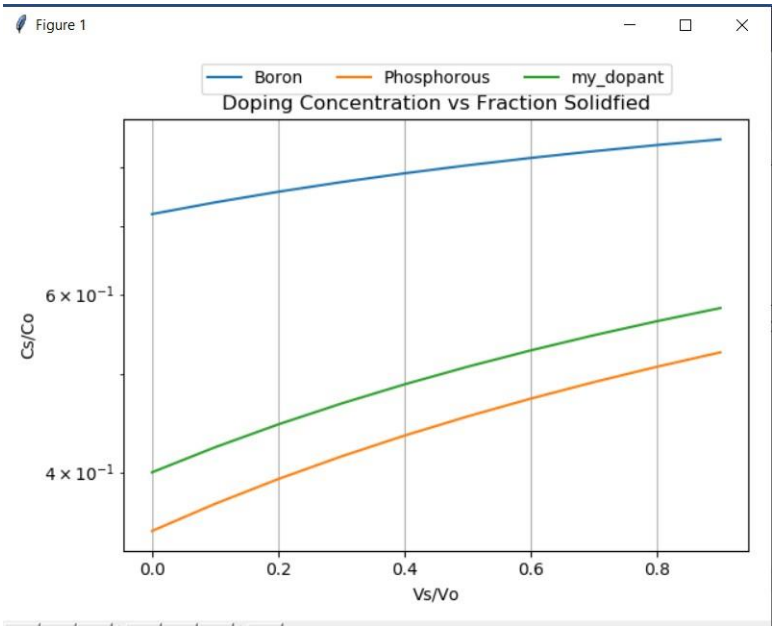


Select atleast one dopant to be plotted. We also have provided an option to enter any custom dopants which are not in the list. For this click on custom option and write its name in enter name option and write its k value that is segregation value. Default name and value is set to Enter name and 1 respectively.

Take a case for Phosphorus, Boron and Custom dopant whose name is my_dopant and whose segregation value is 0.4. Select Phosphorus, Boron and Custom using the checkboxes and click plot.



The following plot is opened,

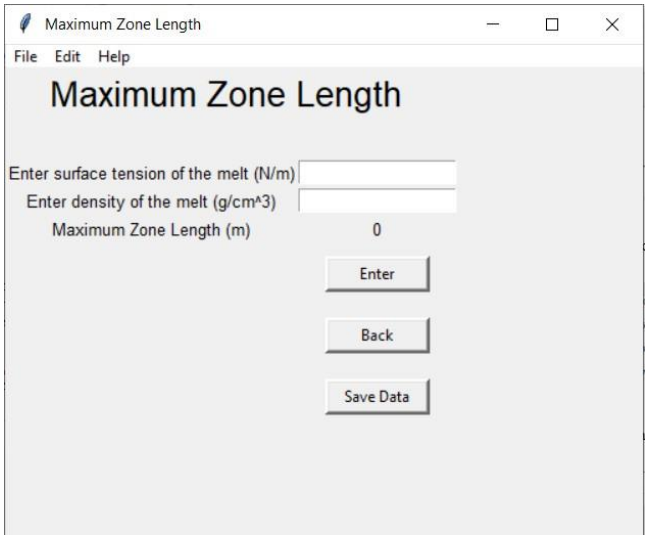


To save the set of data used for plotting, click save data. (Note: Only those data which are plotted will be saved).

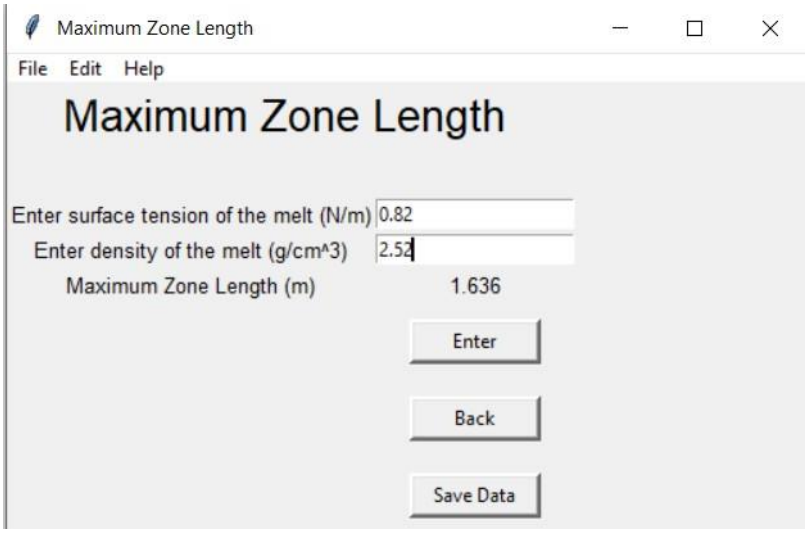
A	B	C	D	E	F	G	H	I	J	K
Fraction Solidfied-->	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Boron (B)	0.72	0.739451	0.757551	0.774394	0.790067	0.804651	0.818221	0.830849	0.8426	0.853535
Phosphorous (P)	0.35	0.372356	0.393944	0.414789	0.434917	0.454353	0.47312	0.491242	0.508741	0.525637
my_dopant	0.4	0.423526	0.44613	0.467848	0.488714	0.508762	0.528023	0.54653	0.564311	0.581394

Maximum Zone Length

To find the **maximum zone length**, select the third option and press select. Following window appears,



Enter some data and press next,

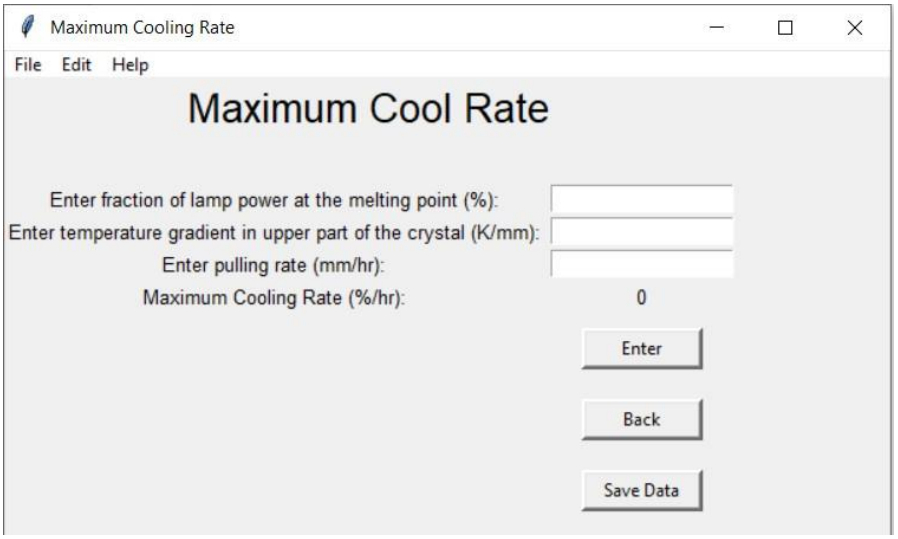


We get the data as 1.636 m. We can save the data for more values, consider different surface tension and density values as (1, 2.32), (0.7, 3). We get the following in csv file.

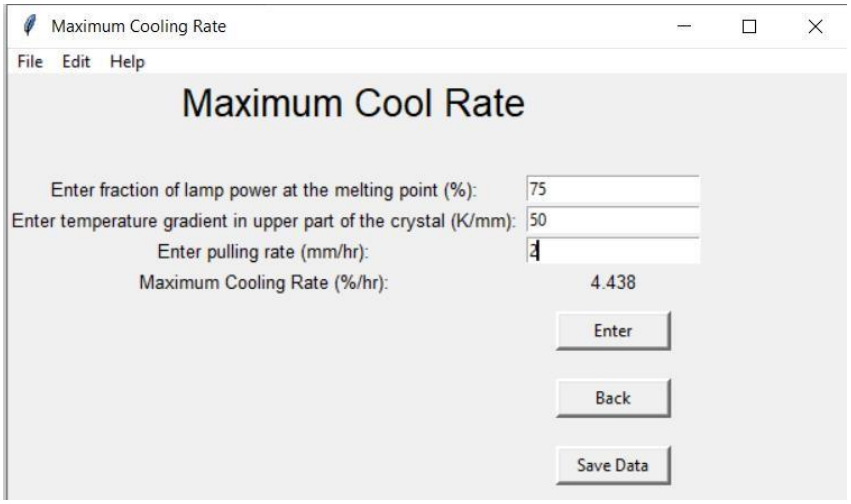
A	B	C
Surface Tension of the Melt (N/m):	Density of the Melt (g/cm^3):	Maximum Zone Length (cm):
0.82	2.52	1.63565043
1	2.32	1.882521062
0.7	3	1.385071615

Maximum Cooling Rate

To find the **maximum cooling rate**, select the fourth option and press select. Following window appears,



Enter some data and press next to get the answer,



We can save the data and get the following in csv file.

A	B	C	D
Fraction of Lamp Power at Melting Point (%)	Temperature Gradient in Upper Part of the Crystal (K/mm)	Pulling Rate (mm/hr)	Maximum Cooling Rate (%/hr)
75	50	2	4.437869822

1.3 Addition Function Description

Some additional functionalities are provided for ease of the user. These functionalities include:

1) Opening a previous saved CSV file

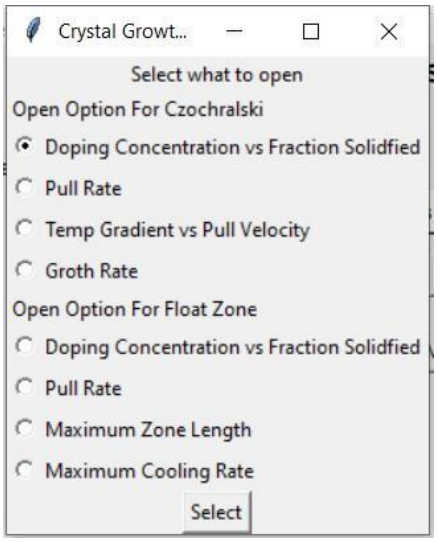
2) Converter

3) Access to manual and formulas used

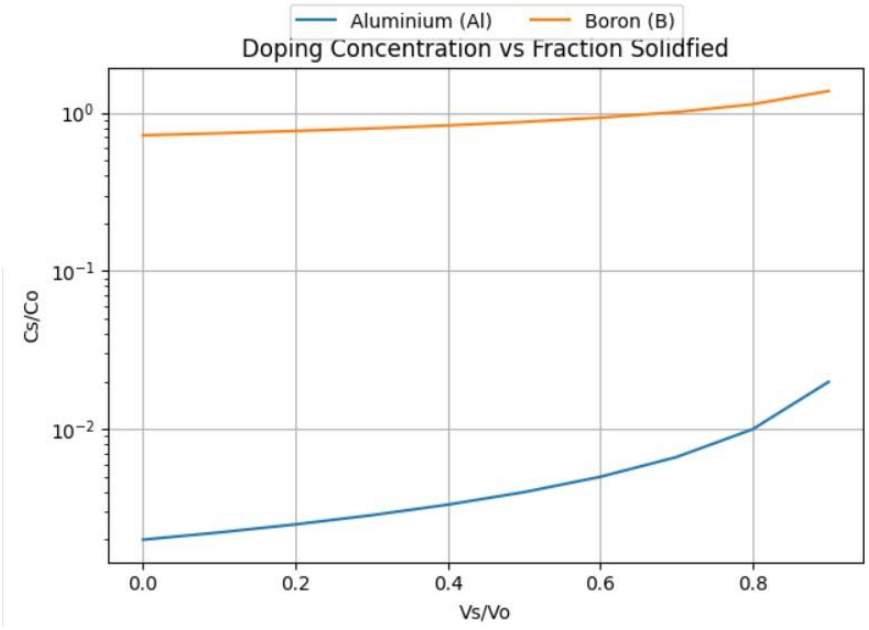
Opening a saved CSV file

The user has the option of opening the saved csv file to see previously saved data or the user can also look at all the currently saved data.

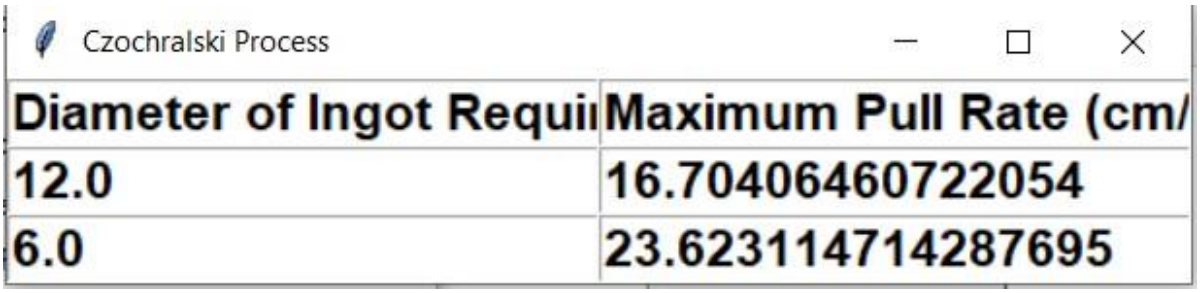
Suppose we want to look at all the data saved in section 3.2, we first go to file menu and select open. Following window opens up,



Select the data you want to see. Suppose we want to re plot all the data in last session, we select doping concentration vs Fraction Solidified and press Select. We get the following plot,



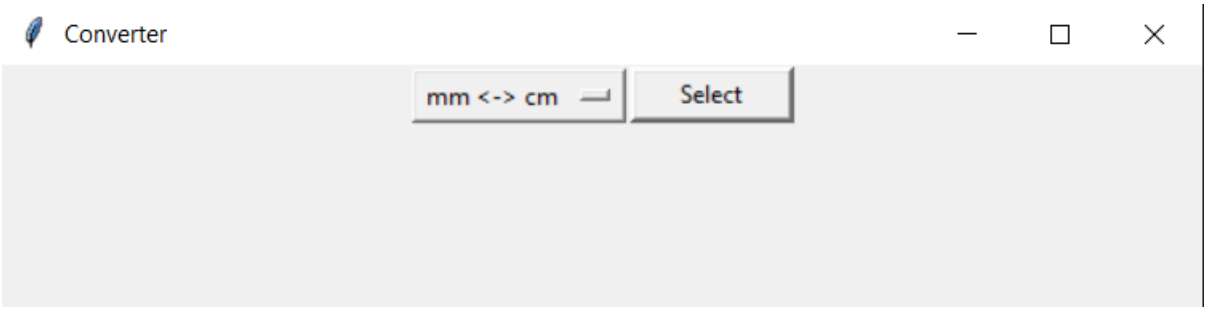
If we open Pull Rate of CZ process,



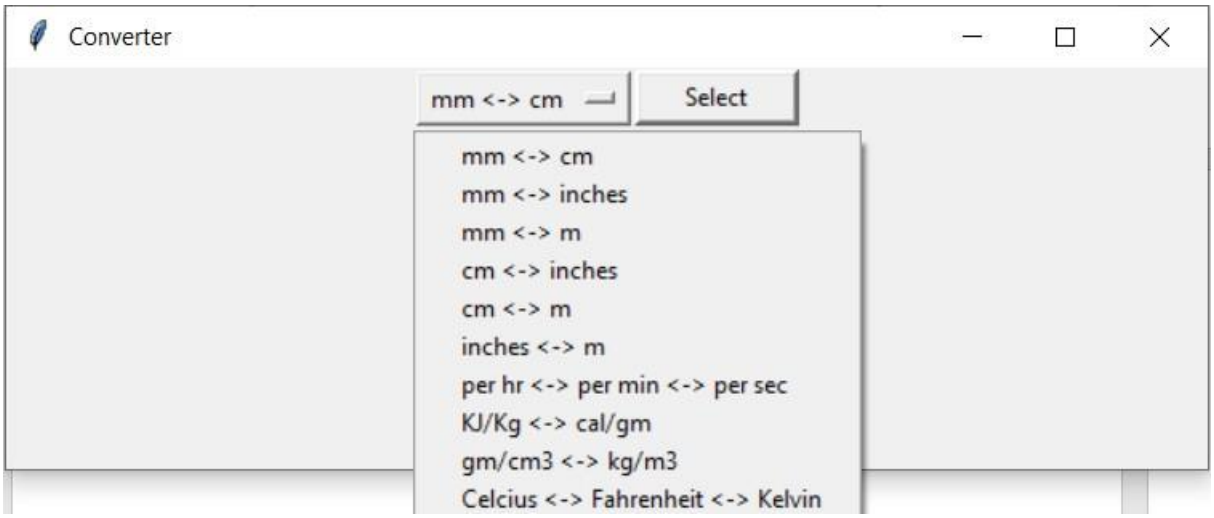
Similarly, all the data can open to see the currently saved or last session saved data. (**Note**: The file will be opened is the format of data is changed or if the file has been renamed. Also, only the data that is saved by pressing the save button will be showed.)

Converter

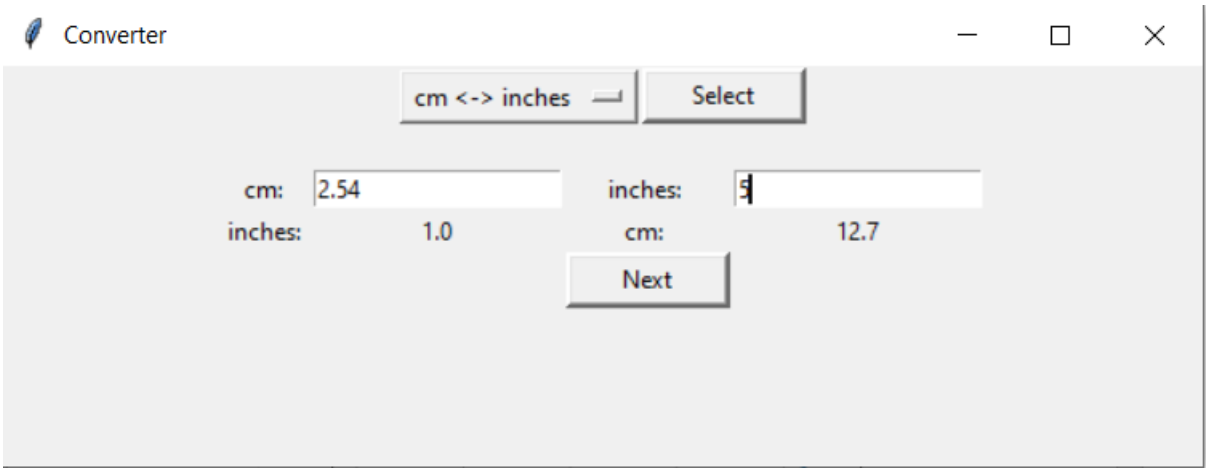
The user is given a converter which can be used to convert some common terms used through out the fields in the tool. Open the converter by clicking on Help menu and select Converter. Following window pops up.



Various options provided are:



For instance, we want to convert between inches and cm, then select cm <-> inches option. Then you will see the following display, enter the details and press next.



Similarly, for other options also, we can calculate our required values.

Access to manual and formulas used

One can access the manual (current pdf) and formulas used from the help menu at the top. A pdf will open showing the required pdf as requested.

(**Note:** The pdf will not open if renamed from default or deleted/moved from its original position.)

2. Examples

Some examples values are provided which are verified using both the tools and hand/manual calculations.

CZ Process - Maximum Pull Rate

Formula used is:

[1].Maximum Pull Rate

$$v_p = \frac{1}{LN}\sqrt{\frac{2\sigma\varepsilon k_M T_M^5}{3r}}$$

Where,

L = Latent Heat of Fusion = 430 cal g^{-1}
N = Density of Silicon = 2.328 gm cm^{-3}
σ = Stefan Boltzmann Constant = 5.67 x 10^{-5} erg cm^{-2} sec^{-1} K^{-4}
Ɛ = Emissivity of Silicon = 0.55
K_M = Thermal Conductivity at T_M = 0.048 cal sec^{-1} cm^{-1} K^{-1}
T_M = Melting Temperature of Silicon = 1690 K
r = Radius of the CZ Crystal

For diameter = 12 inches

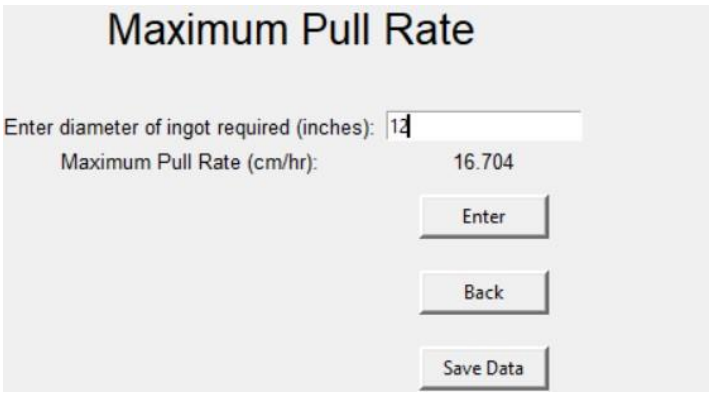
Manual Calculation:

1

$$v_p = \frac{1}{430 * 2.328} \sqrt{\frac{2 * 13.55 * 10^{-13} * 0.55 * 0.048 * 1690^5}{3 * 6 * 2.54}} = 4.636 * 10^{-3} \frac{cm}{s}$$

$$= 16.70 \frac{cm}{hr}$$

Tool Output,



For diameter = 6 inches

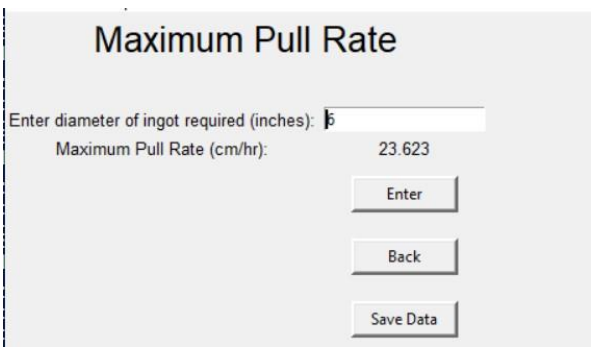
Manual Calculation:

1

$$v_p = \frac{1}{430 * 2.328} \sqrt{\frac{2 * 13.55 * 10^{-13} * 0.55 * 0.048 * 1690^5}{3 * 3 * 2.54}} = 6.556 * 10^{-3} \frac{cm}{s}$$

$$= 23.61 \frac{cm}{hr}$$

Tool Output,



CZ Process – Concentration in Solid Phase vs Fraction Solidified

Formula used for plotting,

[2]. Concentration of Impurity in Solid Phase wrt Fraction Solidifie

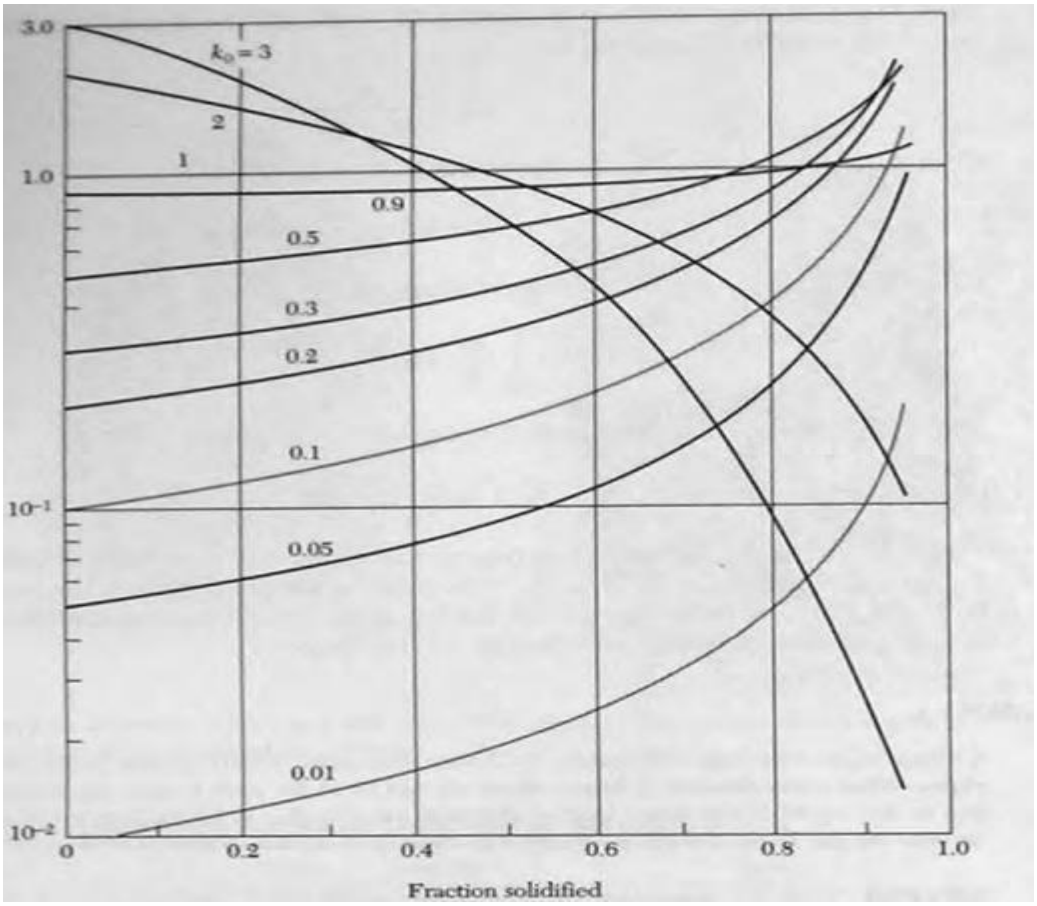
$$C_S = C_O k(1 - f_O)^{1-k}$$

Where,

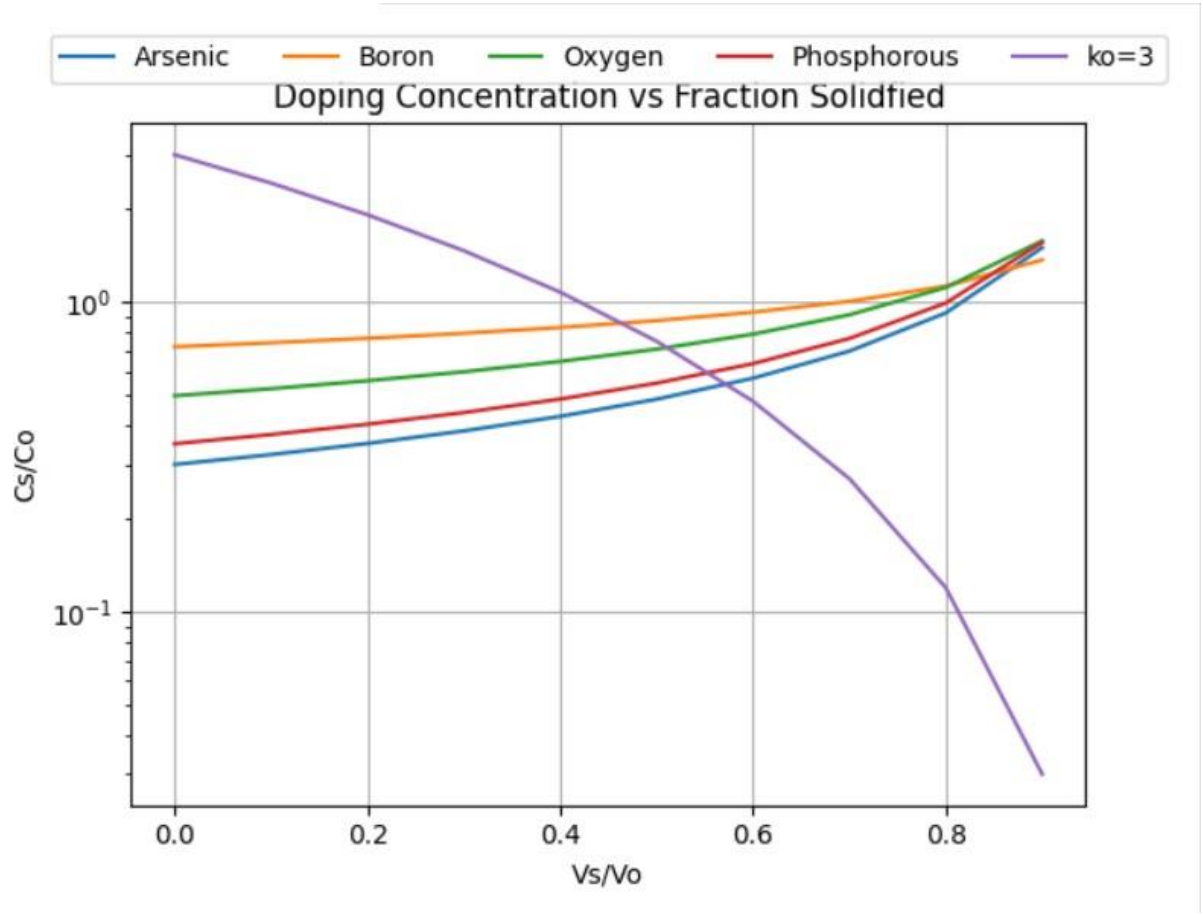
C_s = Concentration of Impurity in Solid Phase =
C_O = Initial Concentration of Impurity
k = Segregation Coefficient
f_o = Fraction Solidified

Segregation Coefficient Table for Silicon	
Impurity	k
Aluminium (Al)	0.002
Antimony (Sb)	0.023
Arsenic (As)	0.3
Boron (B)	0.72
Carbon (C)	0.07
Gallium (Ga)	0.008
Gold (Au)	0.000025
Oxygen (O)	0.5
Phosphorus (P)	0.35

Graph from S.M. Sze Physics of semiconductor devices



Tool Result,



CZ Process – Crystal Growth Rate

Formula used is,

[4]. Crystal Growth Rate

$$f = \frac{v}{1 - \left(\frac{\rho_S}{\rho_m}\right)\left(\frac{D_C}{D_S}\right)^2}$$

Where,

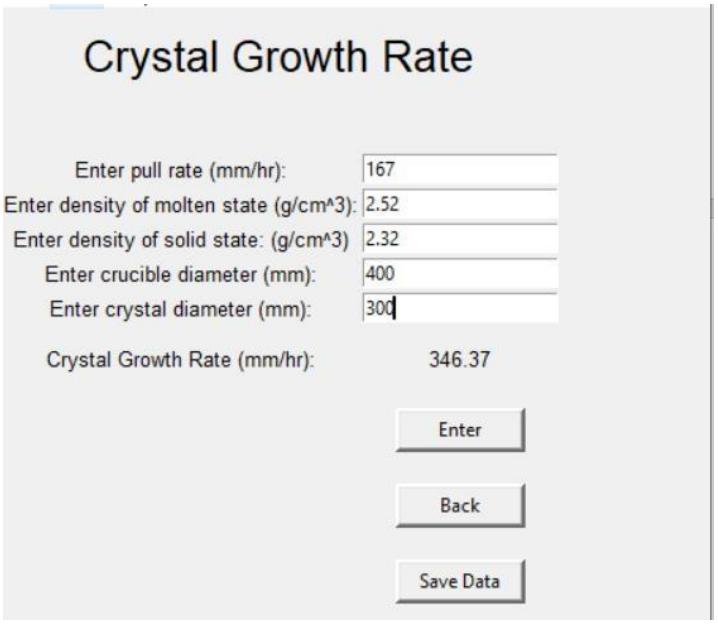
f = Growth Rate (mm hr^{-1})
v = Pull Rate (mm hr^{-1})
ρ_S = Density in Solid State (gm cm^{-3})
ρ_m = Density in Molten State (gm cm^{-3})
D_S = Diameter of crucible (mm)
D_C = Diameter of crystal ingot (mm)

1st Case: For Silicon

Manual Calculation,

$$f = \frac{167}{1 - \left(\frac{2.32}{2.52}\right)\left(\frac{300}{400}\right)^2} = 346.37 \frac{mm}{hr}$$

Tool Result,

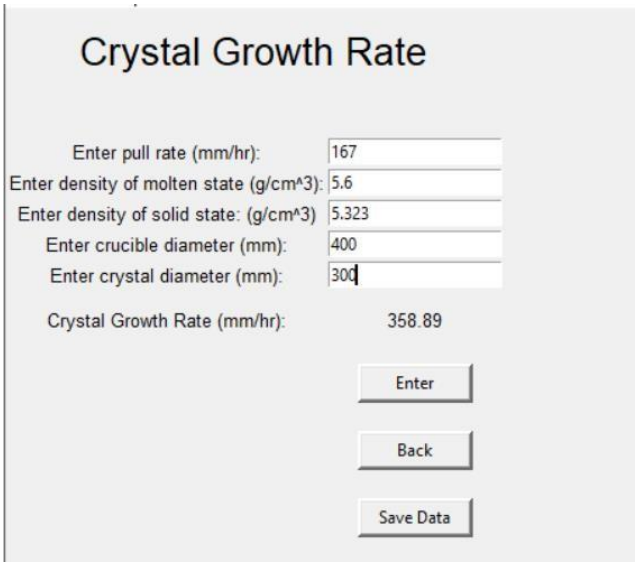


2nd Case: For Germanium

Manual Calculation,

$$f = \frac{167}{1 - \left(\frac{5.323}{5.60}\right)\left(\frac{300}{400}\right)^2} = 358.889 \frac{mm}{hr}$$

Tool Result,



CZ Process – Crystal Growth Rate

Formula used is,

[3]. Temperature Gradient from Solid-Melt Interface

$$G_S = -\frac{\sqrt{8 * B + W^2} - W}{2r}(T - T_a)$$

$$B = \frac{h_a * r}{k}$$

$$W = \frac{C_V * r * v_p}{k}$$

Where,

G_S = Temperature Gradient (°C mm^{-1})
C_V = Specific Heat of Silicon = 0.39 x 10^{-3} J $°C^{-1}$ mm^{-3}
h_a = 6.43 x 10^{-6} W $°C^{-1}$ mm^{-2}
k = Thermal Conductivity = 0.02 W $°C^{-1}$ mm^{-1}
v_p = Pull Velocity (mm min^{-1})
T = Melting Temperature of Silicon = 1400 °C
T_a = Ambient Temperature = 27 °C

Manual Calculation,

Since this calculation considers a range of values of pull rate, we will look at the case for 0 and 0.7 as the value of pull rate for a radius of 150 mm.
For v_p = 0,

$$B = \frac{6.43 * 10^{-6} * 150}{0.02} = 0.048225$$

$$W = 0$$

$$G_S = \frac{\sqrt{8 * 0.048255 + 0} - 0}{2 * 150}(1400 - 27) = 2.842 \ \frac{C}{mm}$$

For v_p = 0.7,

$$B = \frac{6.43 * 10^{-6} * 150}{0.02} = 0.048225$$

$$W = \frac{\frac{0.39 * 10^{-3} * 150 * 0.7}{0.02}}{60} = 0.034125$$

$$G_S = \frac{\sqrt{8 * 0.048255 + 0.034125^2} - 0.034125}{2 * 150}(1400 - 27) = 2.691 \ \frac{C}{mm}$$

Tool Result,

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
Pull Rate (mm/min) -->	0	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95
Temp Gradient (C/mm) for R = 150.0	2.842696	2.820359	2.809256	2.798198	2.787184	2.776215	2.765289	2.754408	2.743571	2.732778	2.722029	2.711324	2.700664	2.690047	2.679475	2.668946	2.658461	2.648021	2.637624

CZ Process – Concentration in Solid Phase vs Fraction Solidified

Formula used for plotting,

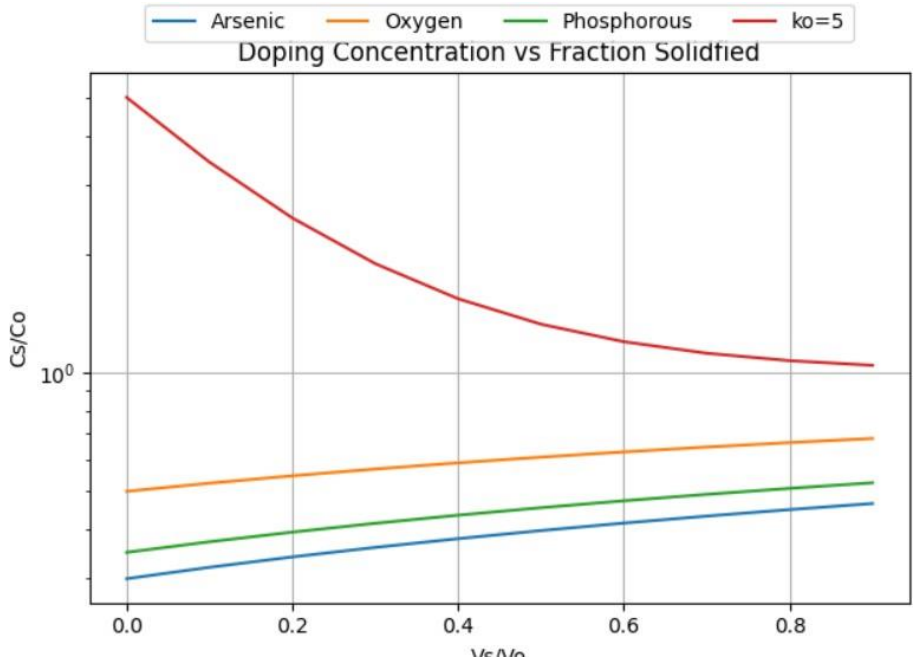
[2]. Concentration of Impurity in Solid Phase wrt Fraction Solidified

$$C_s = C_0[1 - 1(1 - k_e)^{-k_e x/L}]$$

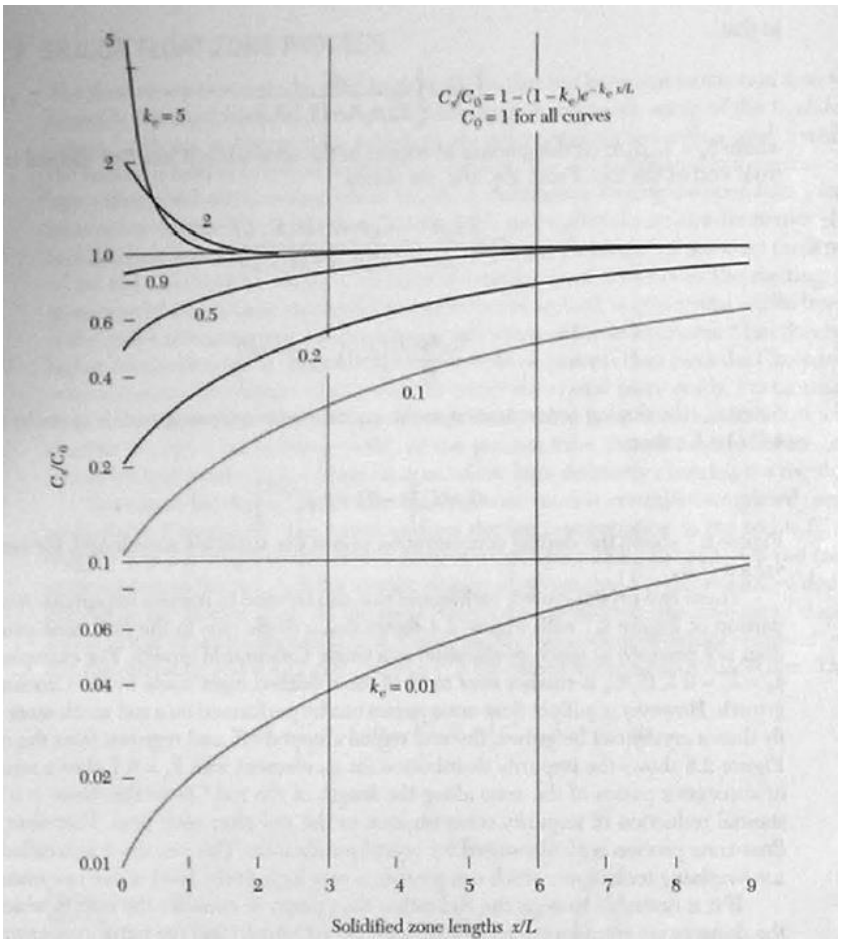
Where,

Cs = Concentration of Impurity in Solid Phase.
CO = Initial Concentration of Impurity.
k_e = Segregation Coefficient
L = Length of the melt zone at a distance x along the rod.

Tool Result,



Graph from S.M. Sze Physics of semiconductor devices



FZ Process – Maximum Zone Length

Formula used is,

[4]. Maximum Float Zone Length

$$L_{max} = 2.84\sqrt{\frac{\sigma}{\rho g}}$$

Where,

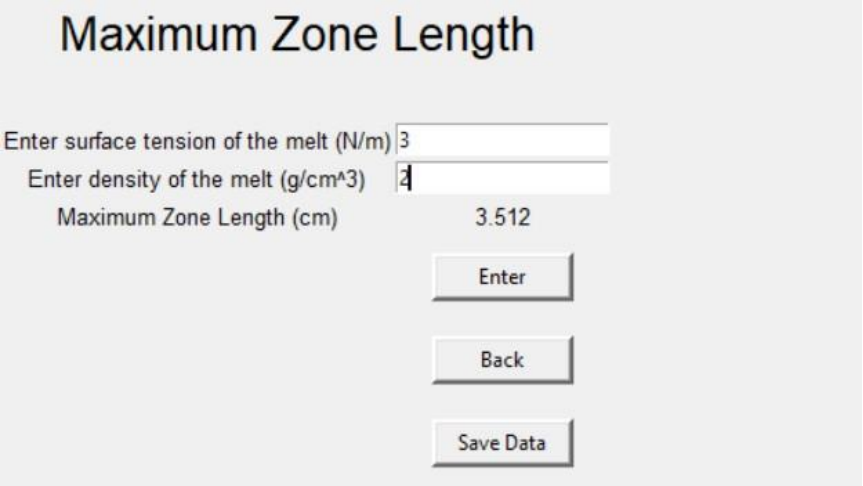
L_{max} = maximum zone length.
σ = surface tension of the melt
ρ = density of the melt.
g = gravity acceleration = 9.8 m sec^{-2}

1st Case: σ = 3 N/m, ρ = 2 gm/cm^3

Manual Calculation,

$$L_{max} = 2.84\sqrt{\frac{3 * 10}{2 * 9.81}} = 3.512\ cm$$

Tool Result,

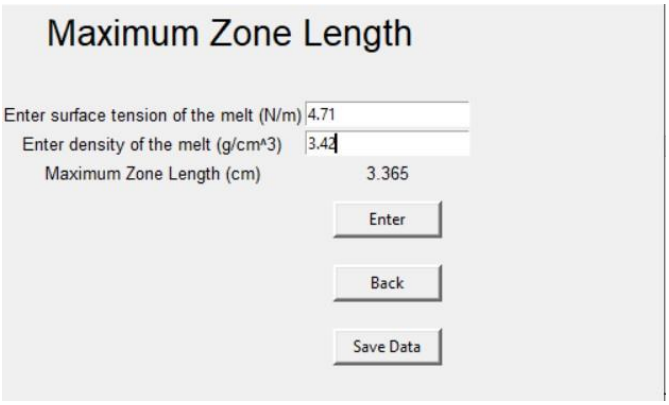


2nd Case: σ = 4.71 N/m, ρ = 3.42 gm/cm^3

Manual Calculation,

$$L_{max} = 2.84\sqrt{\frac{4.71 * 10}{3.42 * 9.81}} = 3.365\ cm$$

Tool Result,



FZ Process – Cooling Rate

Formula used is,

[3]. Maximum Cooling Rate

$$CR = \frac{P_{melt} \cdot \nabla T \cdot v_p}{T_m}$$

Where,

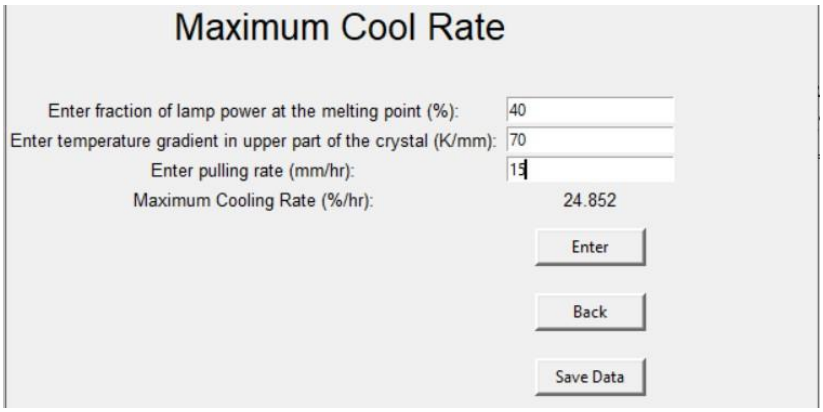
CR = Maximum cooling rate (%/hr)
P_{melt} = Fraction of Lamp power at the melting point.
∇T = Temperature gradient in upper part of the crystal. (50K/mm)
v_p = Pulling rate (mm/hr)
T_m = Melting temperature

1st Case: P_{melt} = 40%, ∇T = 70 K/mm, v_p = 15 mm/hr, T_m = 1690 K

Manual calculation,

$$CR = \frac{40 * 70 * 15}{1690} = 24.852 \frac{\%}{hr}$$

Tool Result,



2nd Case: P_{melt} = 35.42%, ∇T = 27.65 K/mm, v_p = 18.7 mm/hr, T_m = 1690 K

Manual Calculation,

$$CR = \frac{35.42 * 27.65 * 18.7}{1690} = 10.837 \frac{\%}{hr}$$

Tool Result,