CCC REPORT 2013

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Equilibrium Precipitate Model 1.1 Graphical User Interface

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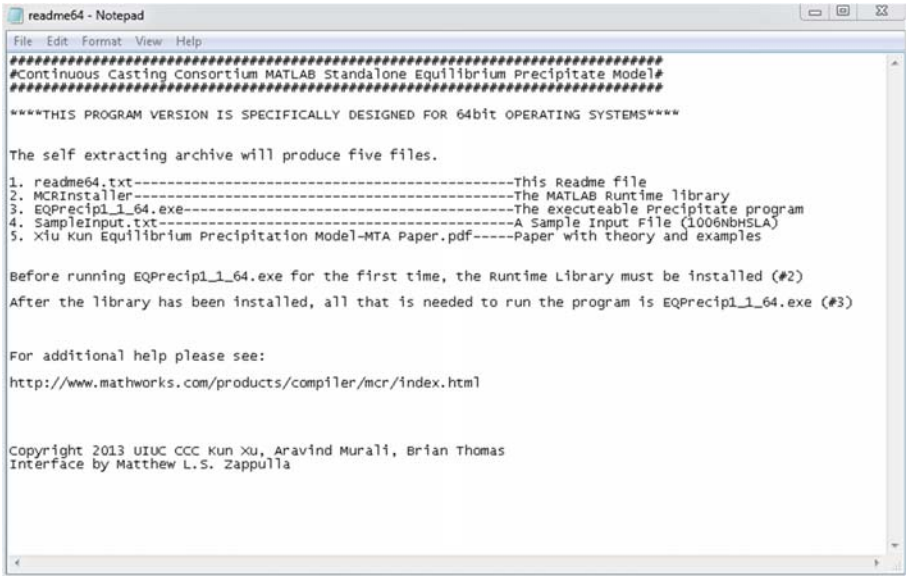
Standalone Program

- **The package includes:**
  - The EQPrecip1.1 exe
  - MATLAB Runtime Library
  - Sample Input File
  - Readme File
  - Supporting Documentation

Name	Type
EQPrecip1_1_64	Application
MCRInstaller	Application
readme64	Text Document
SampleInput	Text Document
Xu Kun Equilibrium Precipitation Model-MTA Paper	Adobe Acrobat Document

- **Once the library is installed, the executable can run**
- **Allows for a smaller program operation**
- **No need for actual MATLAB license**

Installation - Readme File

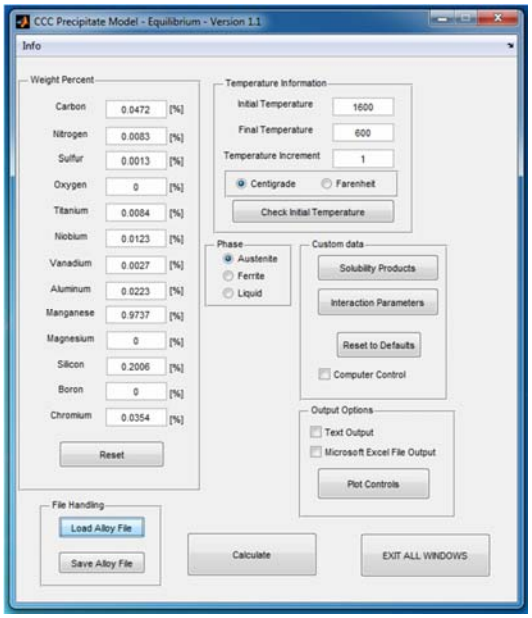


```
readme64 - Notepad
File  Edit  Format  View  Help
##########################################################################
#Continuous Casting Consortium MATLAB Standalone Equilibrium Precipitate Model#
##########################################################################

****THIS PROGRAM VERSION IS SPECIFICALLY DESIGNED FOR 64bit OPERATING SYSTEMS****

The self extracting archive will produce five files.

1. readme64.txt----------------------------------------------This Readme file
2. MCRInstaller----------------------------------------------The MATLAB Runtime library
3. EQPrecip1_1_64.exe----------------------------------------The executeable Precipitate program
4. SampleInput.txt-------------------------------------------A Sample Input File (1006NbHSLA)
5. Xiu Kun Equilibrium Precipitation Model-MTA Paper.pdf-----Paper with theory and examples

Before running EQPrecip1_1_64.exe for the first time, the Runtime Library must be installed (#2)

After the library has been installed, all that is needed to run the program is EQPrecip1_1_64.exe (#3)


For additional help please see:

http://www.mathworks.com/products/compiler/mcr/index.html



Copyright 2013 UIUC CCC Kun Xu, Aravind Murali, Brian Thomas
Interface by Matthew L.S. Zappulla
```

It is important to use the correct version of the program (32bit or 64bit) based on your operating system

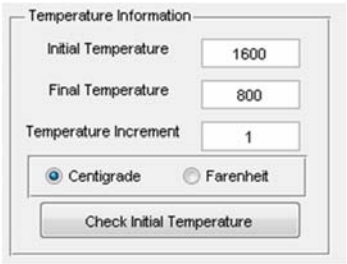
Program Operation

- The program contains default settings with standard options
  - Personalized data or use the program default settings
  - Choice of phases
    - Austenite
    - Ferrite
    - Liquid
  - Temperature data
    - Initial and final temperature
    - Incrementation
    - Computer Check
  - Output of data
    - Excel
    - Text
  - Plot Control Options



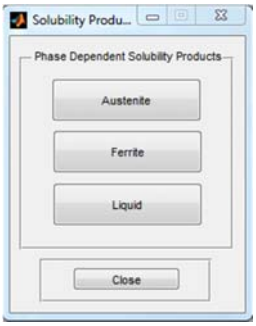
Custom Data

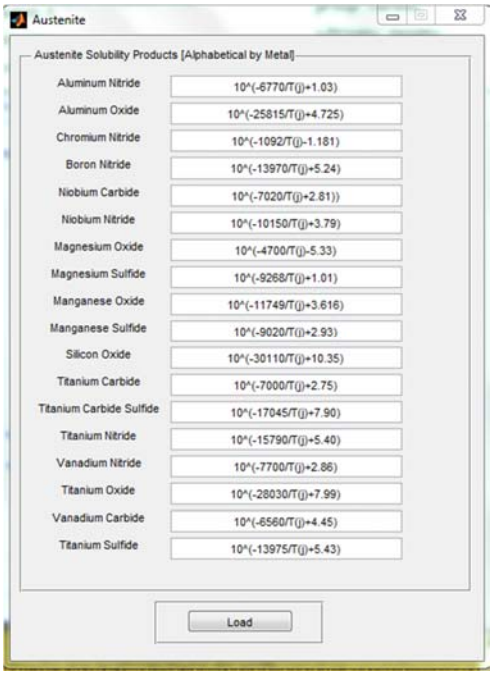
- User has option to enter specific temperature data
- User can also choose automatic computer control of the temperature choices



Solubility Product Options

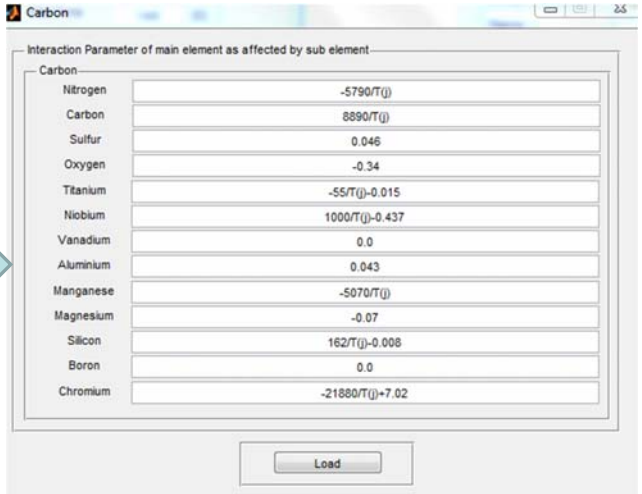
- Choice of custom phase dependent solubility products
  - Select desired phase
  - Adjust solubility product data as desired
  - Load the data
  - Optional Computer Control





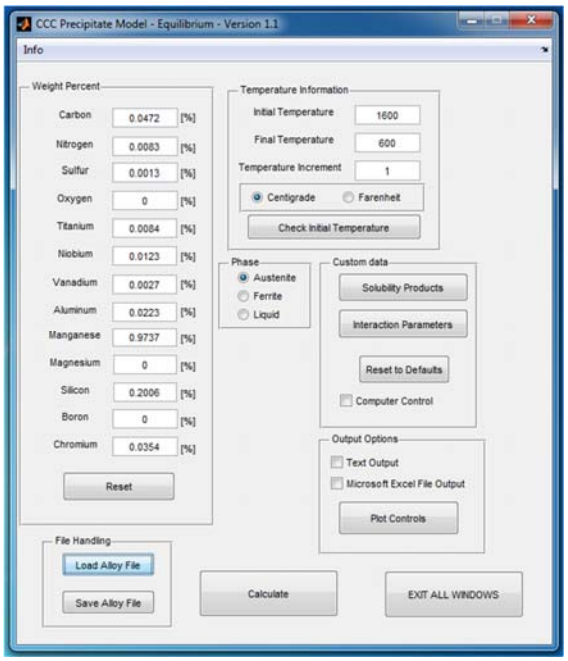
Interaction Parameters

- Element to element interaction parameters
  - Select desired element
  - Adjust interaction parameters as desired



Example Problem - Inputs

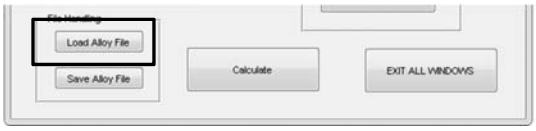
- 0.0472% Carbon
- 0.0083% Nitrogen
- 0.0013% Sulfur
- 0.0% Oxygen
- 0.0084% Titanium
- 0.0223% Aluminum
- 0.9737% Manganese
- 0.2006% Silicon
- 0.0% Boron
- 1600-600°C
  - By 1°C
- Default Behavior
- Output to Excel
- Output to CSV

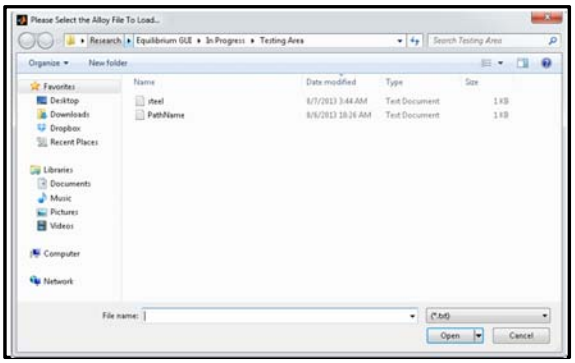


Input Options – Input Files

- Reload old saved cases right back into the program
- Type up an alloy composition in a text editor
- Changes the output file default names automatically to track different cases

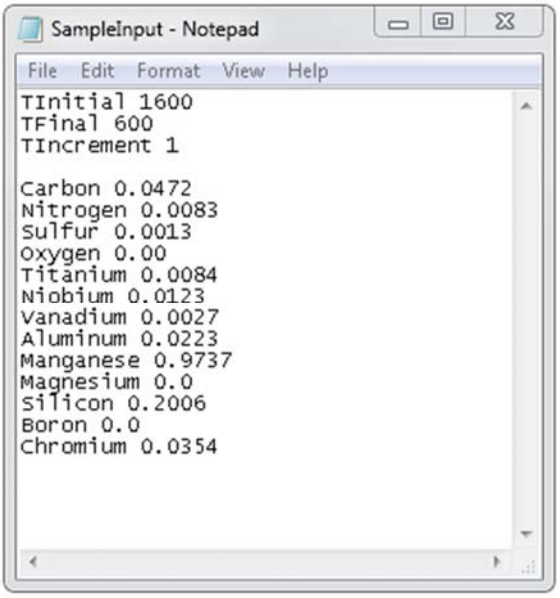
On Button Selection ⇨ File Navigation ⇨ File Selection





Example Problem – Input File

- Load All Program Behavior From File
  - 0.0472% Carbon
  - 0.0083% Nitrogen
  - 0.0013% Sulfur
  - 0.0% Oxygen
  - 0.0084% Titanium
  - 0.0223% Aluminum
  - 0.9737% Manganese
  - 0.2006% Silicon
  - 0.0% Boron
  - 1600-600°C
    - By 1°C
  - Default Behavior
  - Output to Excel
  - Output to CSV



SampleInput - Notepad

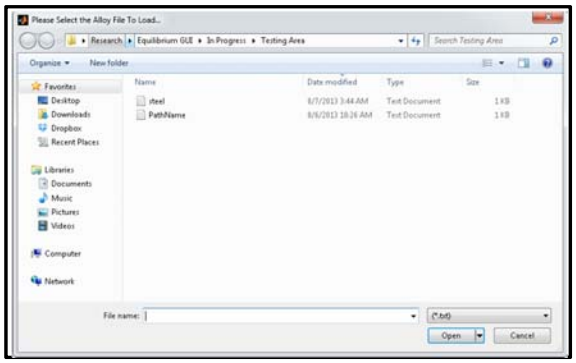
File Edit Format View Help

```
TInitial 1600
TFinal 600
TIncrement 1

Carbon 0.0472
Nitrogen 0.0083
Sulfur 0.0013
Oxygen 0.00
Titanium 0.0084
Niobium 0.0123
Vanadium 0.0027
Aluminum 0.0223
Manganese 0.9737
Magnesium 0.0
Silicon 0.2006
Boron 0.0
Chromium 0.0354
```

Input Options – Save Input Files

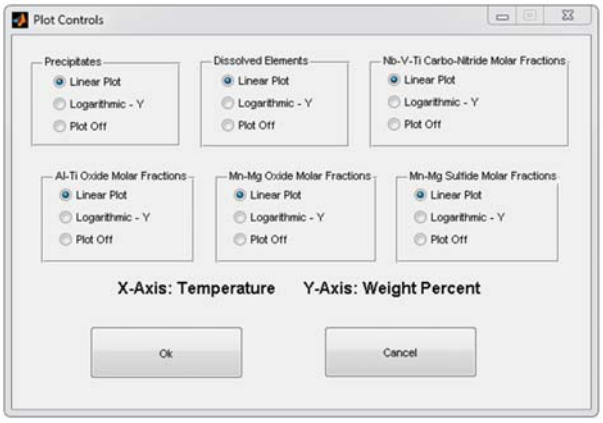
- Save your cases in repeatable easy to read format
- Load right back into the program
- Text editor friendly

On Button Selection ⇨ File Navigation ⇨ File Selection



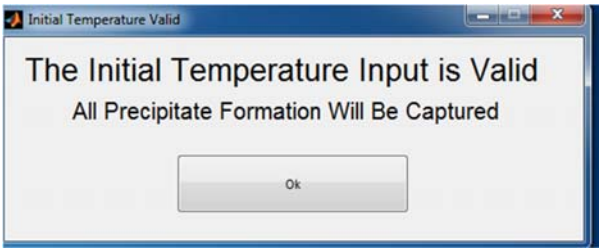
Output Options – Plot Controls

- Choice of Plots
  - Precipitates (by wt%)
  - Dissolved Elements (by wt%)
  - Nb-Ti-V Nitride Molar Fractions
  - Al-Ti Oxide Molar Fractions
  - Mn-Mg Oxide Molar Fractions
  - Mn-Mg Sulfide Molar Fractions
- Choice of Plot Output Type
  - Linear (default)
  - Logarithmic Y-Axis
- Suppress Individual Plots Completely



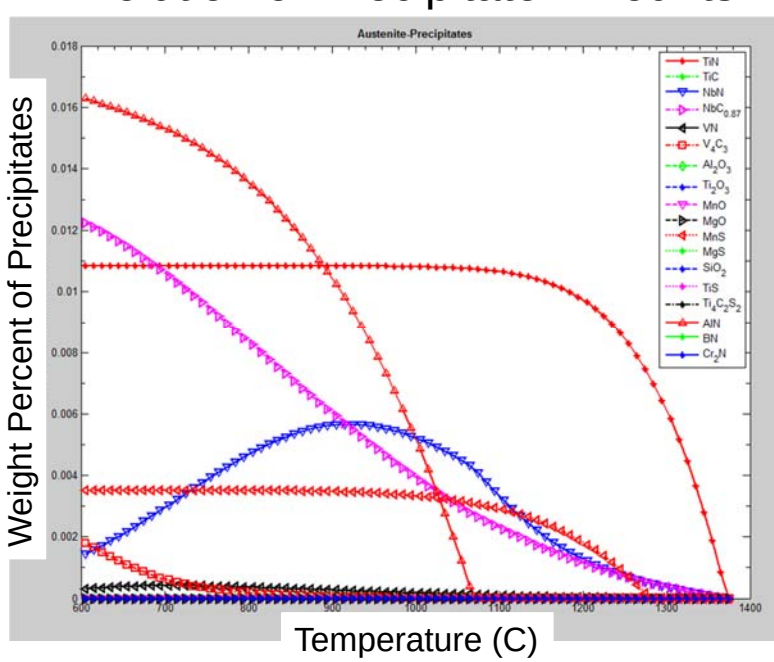
Temperature Check

- Before Executing, The program will verify that the supplied temperature range will capture all precipitate formation
- If the supplied range is not sufficient, the program alerts the user to the precipitation temperature and executes with the proper temperature range



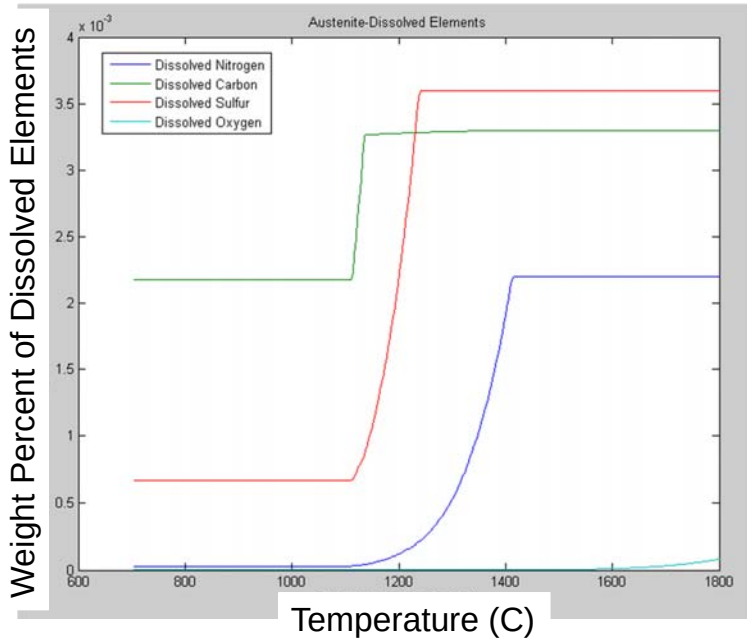
Example Problem – Output Plots

Evolution of Precipitate Amounts



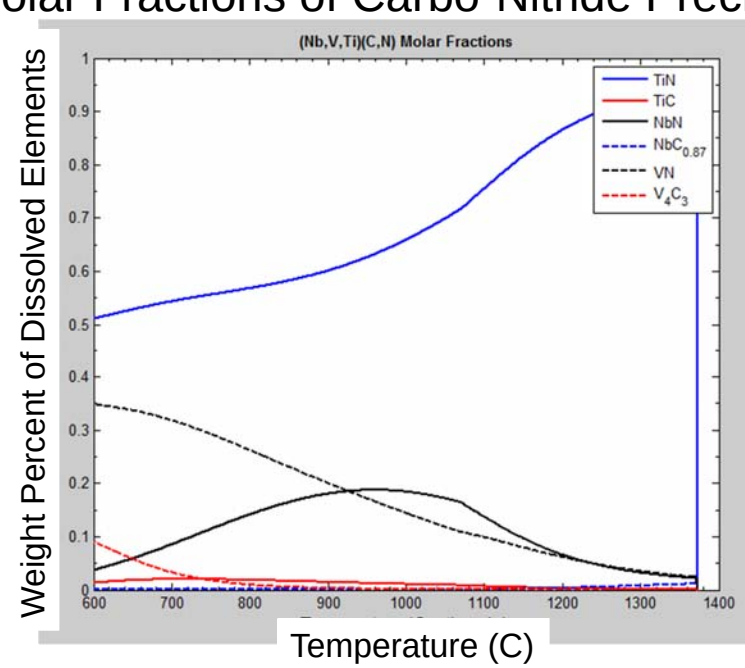
Example Problem – Output Plots

Evolution of Dissolved Elements (N,C,S,O)



Example Problem – Output Plots

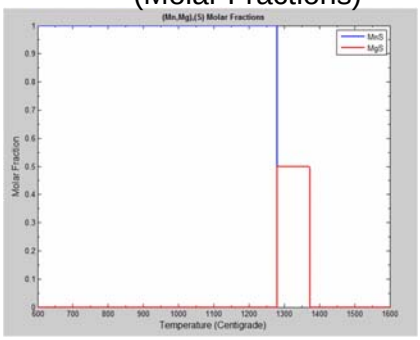
Molar Fractions of Carbo-Nitride Precipitates



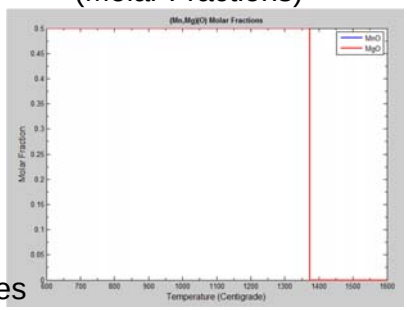
(Nb,V,Ti)(C,N)

Example Problem – Output Plots

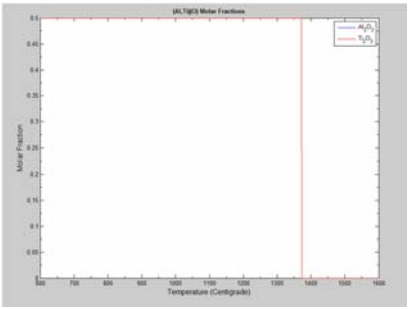
Mn and Mg Sulfide Precipitates
(Molar Fractions)



Mn and Mg Oxide Precipitates
(Molar Fractions)

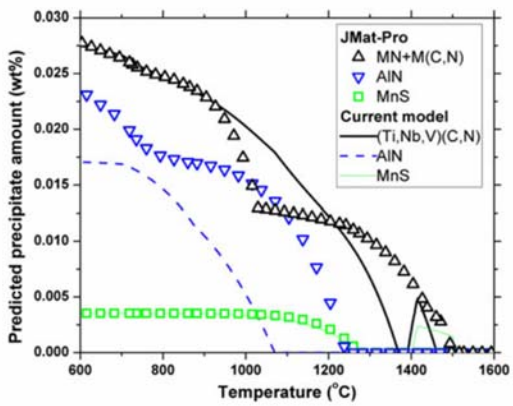


Al and Ti Oxide Precipitates
(Molar Fractions)

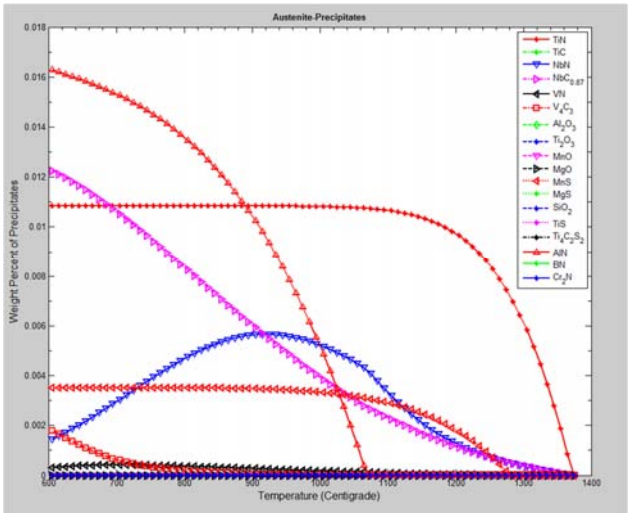


Program Comparison – Example Problem

JMAT Pro



EQPrecip1.1

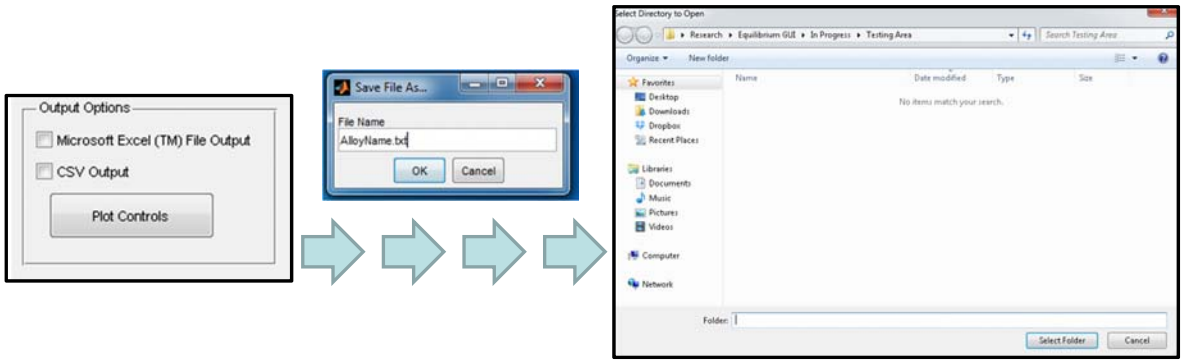


Evolution of Precipitate Amounts (wt%)

Output Options – Output Files

- Choice of Output File Types
  - Excel as a .xls
  - Text as a .txt
- Filename based off of input filename (if used)

On Checkbox Selection ⇨ Filename Selection ⇨ File Save Location Selection



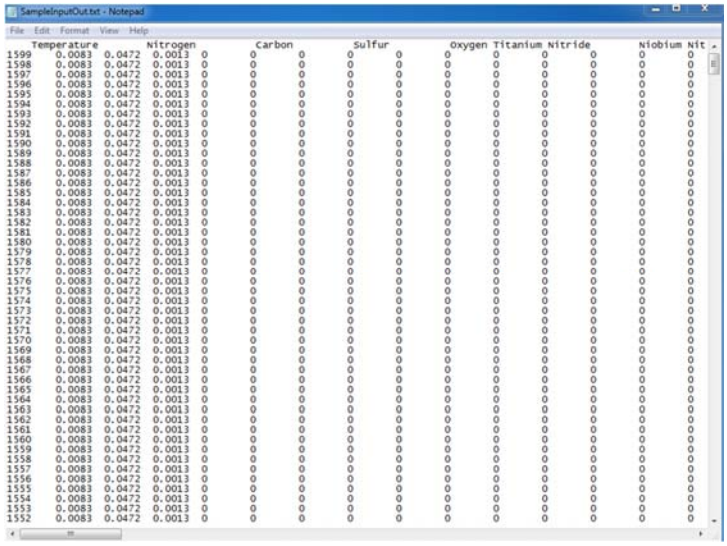
Ex Problem Output - .xls

- The Output to excel option generates a detailed spreadsheet
  - Each precipitate is given in a column in relation to the temperature column to the left
  - If a precipitate is not present it does not appear, this makes reading the spreadsheet much easier

Temperature	Dissolved Nitrogen	Dissolved Carbon	Dissolved Sulfur	Titanium Nitride	Titanium Carbide	Noibium Nitride	Niobium Carbide
1600	0.0083	0.0472	0.0013	0	0	0	0
1599	0.0083	0.0472	0.0013	0	0	0	0
1598	0.0083	0.0472	0.0013	0	0	0	0
1597	0.0083	0.0472	0.0013	0	0	0	0
1596	0.0083	0.0472	0.0013	0	0	0	0
1595	0.0083	0.0472	0.0013	0	0	0	0
1594	0.0083	0.0472	0.0013	0	0	0	0
1593	0.0083	0.0472	0.0013	0	0	0	0
1592	0.0083	0.0472	0.0013	0	0	0	0
1591	0.0083	0.0472	0.0013	0	0	0	0
1590	0.0083	0.0472	0.0013	0	0	0	0
1589	0.0083	0.0472	0.0013	0	0	0	0
1588	0.0083	0.0472	0.0013	0	0	0	0
1587	0.0083	0.0472	0.0013	0	0	0	0
1586	0.0083	0.0472	0.0013	0	0	0	0
1585	0.0083	0.0472	0.0013	0	0	0	0
1584	0.0083	0.0472	0.0013	0	0	0	0
1583	0.0083	0.0472	0.0013	0	0	0	0
1582	0.0083	0.0472	0.0013	0	0	0	0
1581	0.0083	0.0472	0.0013	0	0	0	0
1580	0.0083	0.0472	0.0013	0	0	0	0
1579	0.0083	0.0472	0.0013	0	0	0	0
1578	0.0083	0.0472	0.0013	0	0	0	0
1577	0.0083	0.0472	0.0013	0	0	0	0
1576	0.0083	0.0472	0.0013	0	0	0	0
1575	0.0083	0.0472	0.0013	0	0	0	0
1574	0.0083	0.0472	0.0013	0	0	0	0
1573	0.0083	0.0472	0.0013	0	0	0	0
1572	0.0083	0.0472	0.0013	0	0	0	0

Ex Problem Output - .txt

- The Output to text option generates a detailed space delimited txt file
- Each precipitate is given in a column in relation to the temperature column to the left



SampleInputOut.txt - Notepad

File Edit Format View Help

	Temperature		Nitrogen		Carbon		Sulfur		Oxygen	Titanium	Nitride		Niobium	Nit
1599	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1598	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1597	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1596	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1595	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1594	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1593	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1592	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1591	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1590	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1589	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1588	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1587	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1586	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1585	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1584	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1583	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1582	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1581	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1580	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1579	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1578	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1577	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1576	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1575	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1574	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1573	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1572	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1571	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1570	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1569	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1568	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1567	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1566	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1565	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1564	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1563	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1562	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1561	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1560	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1559	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1558	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1557	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1556	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1555	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1554	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1553	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0
1552	0.0083	0.0472	0.0013	0	0	0	0	0	0	0	0	0	0	0

Acknowledgments

- Continuous Casting Consortium Members (ABB, ArcelorMittal, Baosteel, Magnesita Refractories, Nippon Steel and Sumitomo Metal Corp., Nucor Steel, Postech/ Posco, Severstal, SSAB, Tata Steel, ANSYS/ Fluent)
- Kun Xu, PhD.
- Aravind Murali
- Prof. Brian Thomas