Computation of Pseudo-Binary Phase Diagrams for Dissimilar Metal Welds

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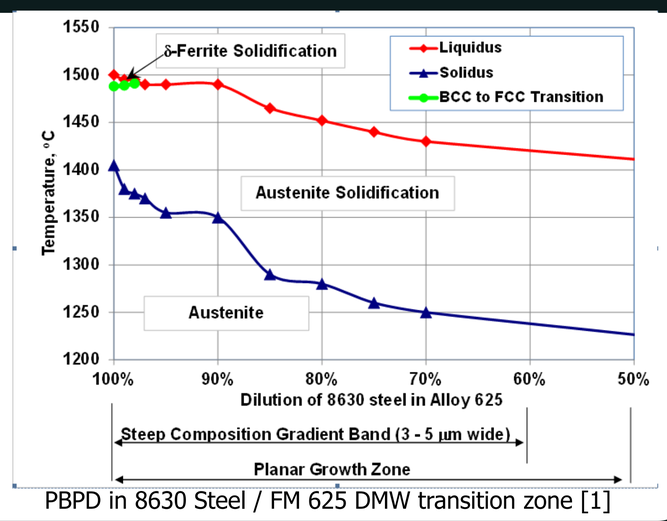
Background

Pseudo Binary Phase Diagrams (PBPDs) were originally developed to study the solidification behavior, including solidification temperature range and solidification mode, in the transition zone of Dissimilar Metal Welds (DMWs) between steel base metals and Ni-base filler metals [1]. PBPDs have been subsequently employed in studies of solidification cracking susceptibility, shrinkage porosity, and partitioning of alloying elements in various DMWs in relation to materials selection and process optimization [2, 3, 4].

PBPDs were originally developed by performing thermodynamic simulations of non-equilibrium solidification, utilizing the Scheil-Gulliver module of ThermoCalc™, at 5% to 10% dilution steps between the base metal and filler metals. The phase transformation data were manually extracted form the ThermoCalc™ solutions and plotted for the entire dilution range from 0 to 100% dilution. The PBPD development procedure required the user to:

- Generate and save a script file and run it within ThermoCalc™
- Save the resulting diagram and extract values where each different phase begins
- Record that data in an organized excel spreadsheet

And even then most PBPDs are created with dilution steps of 10% from 0 to 100, possibly missing phases in between.



PBPD in 8630 Steel / FM 625 DMW transition zone [1]

Motivation

The original methodology for development of Pseudo Binary Phase Diagrams is time consuming and inefficient. The large dilution steps of 5% to 10% may result in inaccurate results and omission of some phase transformations. Improving the process for generation of PBPDs would allow faster and more efficient analyses of DMWs, processing of large databases, and implementation in alloy development.

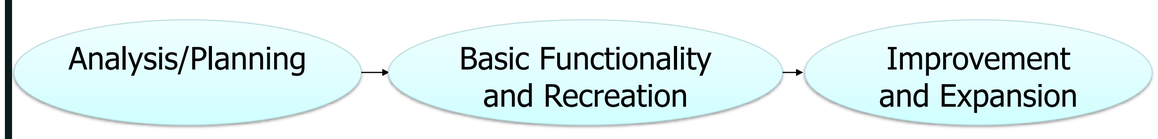
Objectives & Approach

Objectives:

1. Analyze the process of PBPD creation to determine what aspects of the development can be improved upon
2. Recreate the process with a program capable of replicating results created by the original method
3. Automate the process with the main goal of greatly decreasing the amount of time it takes to generate results without losing accuracy
4. Add additional functionality of Partitioning Coefficients and Equilibrium Pseudo Binary Phase Diagrams to allow for extensive analyses of DMWs, including post weld heat treatment

Approach:

- After becoming familiar with the PBPD creation, use TCPython, a Python library containing every capability of ThermoCalc™, to recreate and automate the process of PBPD development.



Conclusions

- The PBPD Automation Code decreases the time for PBPDs creation from several hours for manually generated diagrams with 10% dilution step to approximately 30 minutes of automated generation with 1% dilution step.
- This process also includes the graphs being saved, including the partitioning coefficients, as well as the recording of the data and plotting within Excel, which was a particularly time-consuming part of the original process.
- The PBPD Automation Code allows for efficient processing of large databases of base metal / welding filer metal combinations and is applicable for materials selection, materials development, and process optimization for DMWs.

Future Work

- Improvements to the user interface to make the application easier to use.
- Adapting the code to future projects on alloy development and optimization.
- Working with ThermoCalc to potentially include the functionality of this project within ThermoCalc's flagship program.
- Software update's and quality of life improvements.

Results & Discussion

PBPD Automation

- Created a program called PBPD Automation which requires a lot of input from the user to run simulations
- Greatly decreases the amount of time taken to make PBPD

Scheil Simulations

- PBPD Automation runs as many Scheil simulations at any dilutions mixes that the user wants and plots them
- Automation allows for much more data to be recorded, possibly finding more phase than manual

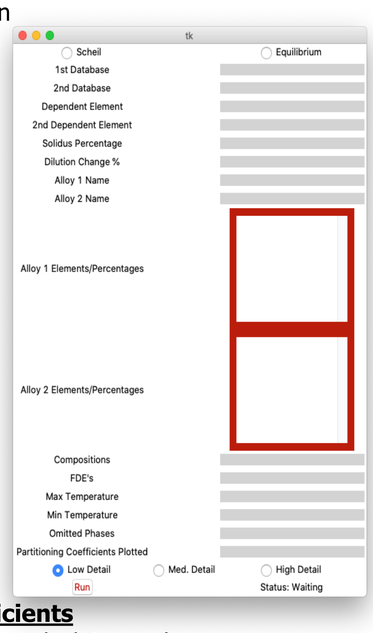


Figure: Generated Scheil simulation data from PBPD Automation with a dilution step of 1%

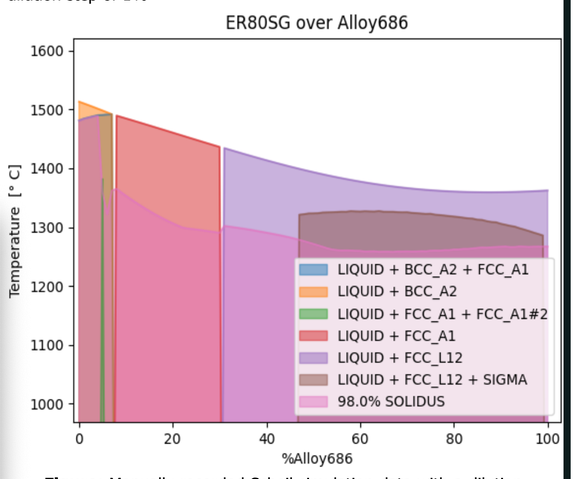
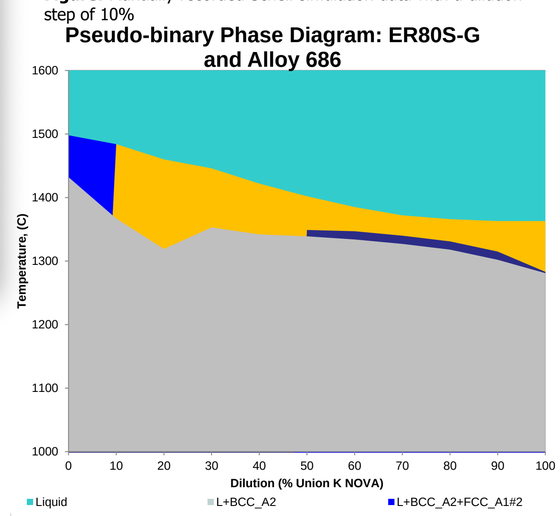


Figure: Manually recorded Scheil simulation data with a dilution step of 10%



Partitioning Coefficients

- The software also calculates and records partitioning coefficients for elements within the alloy
- The user chooses which elements to record partitioning coefficient data for

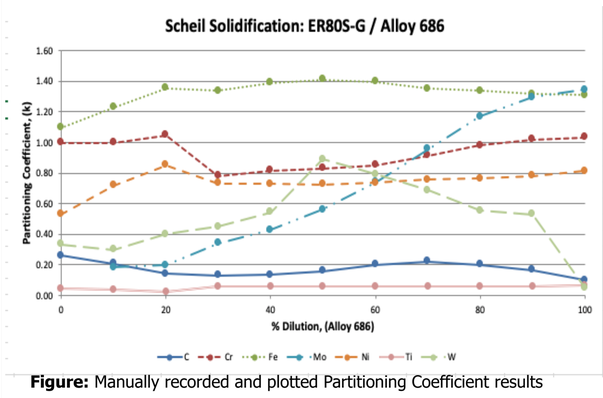


Figure: Manually recorded and plotted Partitioning Coefficient results

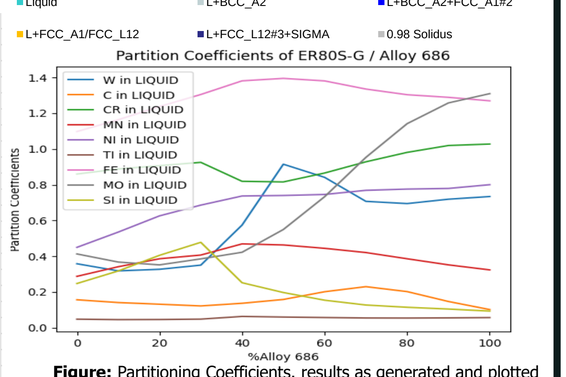


Figure: Partitioning Coefficients. results as generated and plotted by PBPD Automation

Equilibrium Diagrams

- PBPD Automation is also capable of creating Equilibrium diagrams

Figure: Manually generated Equilibrium Diagram with a dilution step of 10%

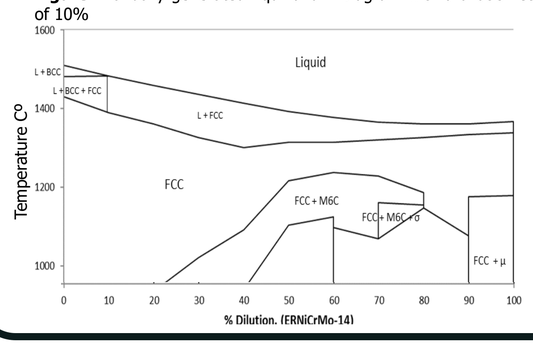
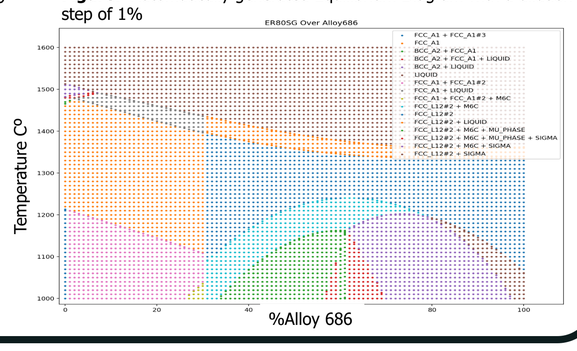


Figure: Automatically generated Equilibrium Diagram with a dilution step of 1%



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