

JMatPro® API with THERCAST® 9.0

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JMatPro® software

Introduction

From their website¹, it is defined by:

JMatPro® is a simulation software which calculates a wide range of materials properties for alloys and is particularly aimed at multi-components alloys used in industrial practice.

Using JMatPro® you can make calculations for:

- Stable and metastable phase equilibrium
- Solidification behaviour and properties
- Mechanical properties
- Thermo-physical and physical properties
- Phase transformations
- Chemical properties

¹<http://www.sentessoftware.co.uk/jmatpro.aspx>

Simulation data given by JMatPro®

JMatPro® databases give access to (at a given composition or temperature):

- ① **Thermodynamic** data for each phase: *volume/mass fraction, composition, density, enthalpy ...*
- ② **Thermophysical** data: *fraction, composition, density, enthalpy ...*
- ③ **Thermomechanical** data: *viscosity, surface tension, bulk and shear moduli ...*
- ④ **Electrical** data: *Electrical conductivity/resistivity ...*

Technical limitations and drawbacks

- Like any thermodynamic software, you should **know** what to **expect** :-)
- Software specificities: σ -phase precipitates are available in stainless steels but not in general steels (check χ -phase)
- According to the product flyer, metastable phases are only available with Al alloys
- Other ? (For now it is not easy to know more, I need to dig in deeper ...)

JMatPro® GUI

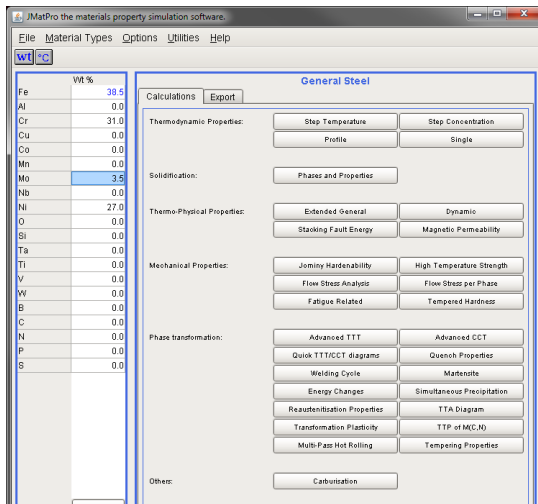
Intro

At TSV, it is only used via the interface (with only one machine-license)



Intro (contd)

Several modules are available through the “Material Types” tab then choosing any material (**General Steel** in this case)



Data validation

Testing Solidification module with **General Steels**

The Solidification module features a 0D computation^a

^a<http://www.sentessoftware.co.uk/jmatpro.aspx>

2: assumed at a point

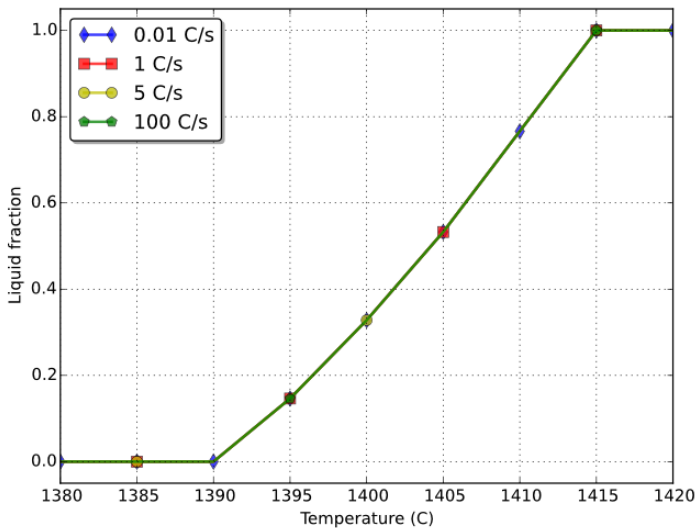



Figure 3: Solidification paths plots at nominal composition (UR28-Quatern) for several

Limitations related to the GUI

- ① Predefined exports: user is limited to available data exports, therefore no possibility to readily customize output
- ② Input parameters may change for the same module if the material changes, with no documentation of the models using them:
 - Input parameters for **General** steels in Solidification are: grain size (μm) , initial temperature³(°C) and cooling rate (°C/s) => related to a *Kirkaldy* model ?
 - Input parameters for **Stainless** steels in Solidification are: initial temperature⁴(°C) and minimum liquid fraction (-) => related to a *Scheil-Gulliver* model ?
- ③ It is not possible to choose phases for **General** steels in Solidification
- ④ The modified⁵ Gulliver-Scheil model is not an option in the interface
- ⑤ other ?

³above nominal liquidus

⁴above nominal liquidus

⁵allowing fast diffusion for interstitial elements, carbon and nitrogen 

JMatPro® API

API vs GUI

The API offers immediate advantages over the interface :

- Extend, organise, process and format output as needed ==> customised data export
- Seamless implementation with existing tools
- Automate batch data generation (e.g. vary nominal composition with temperature stepping)
- Combine functionalities from different modules (e.g. Solidification and Thermodynamic Properties)

API components/modules

From the API documentation⁶

- **Core:** provides core functionality and contains functions used for general settings, or for settings which are common to several modules.
- **Solver:** provides functions to set up and run thermodynamic calculations of stable and metastable phase equilibria in multicomponent alloys, as well as nonequilibrium Scheil-Gulliver calculations.
- **Coldfire:** allows for the calculation of physical, thermophysical, and room-temperature matrix mechanical properties.
- **Solidification:** provides functions to set up and run calculations of phase evolution, as well as physical and thermophysical properties, during solidification.
- **TTT:** allows for the calculation of time-temperature transformation (TTT) diagrams of general steels.
- **CCT:** allows for the calculation of continuous cooling transformation (CCT) diagrams of general steels.

⁶<http://www.sentessoftware.co.uk/jmatpro.aspx>

API components/modules : Core module

Core functions like `jmpSetMaterialType` and `jmpSetAlloyComposition` are compulsory for any program using the API. Available (compulsory and optional) functions in the module:

API components/modules : Solver module

Solver is the most important module in the API. It contains the necessary routines to perform general thermodynamic calculations at equilibrium and non-equilibrium. This module will be my point of interest for the segregation functionality in THERCAST®. Available functions in the module:

API drawbacks

- No getter functions are available in the API, results are hard-written in *.out files
- other ?

Reference Guide (links to official API documentation)

API documentation : Core module

- `jmpSetWorkingDirectory()`
- `jmpSetScreenOutput()`
- `jmpSetMaterialType()`
- `jmpSetAlloyElements()`
- `jmpSetCompositionUnit()`
- `jmpSetAlloyComposition()`
- `jmpSetFastInterstitial()`
- `jmpSetFerriteCheck()`
- `jmpSetTemperatureUnit()`
- `jmpSetAustenitisationTemperature()`
- `jmpSetGrainSizeUnit()`
- `jmpSetAusteniteGrainSize()`
- `jmpSetStartTransformationFraction()`

API documentation : Solver module

- `jmpSetSolverCalculationType()`
- `jmpSetSolverTemperature()`
- `jmpSetMultiplePoints()`
- `jmpSetTemperatureStepping()`
- `jmpSetExtendedStepping()`
- `jmpSetConcentrationStepping()`
- `jmpSetBalancing()`
- `jmpSetScheilFractionLimit()`
- `jmpSetSolverPhases()`
- `jmpSetDefaultPhases()`
- `jmpExcludeSolverPhases()`
- `jmpSetPhaseStatus()`
- `jmpSetPhaseBoundariesSearch()`
- `jmpRunSolverCalculation()`

API documentation : Coldfire module

- `jmpSetColdfireCalculationType()`
- `jmpSetPhysicalProperty()`
- `jmpUnsetPhysicalProperty()`
- `jmpSetMechanicalProperty()`
- `jmpUnsetMechanicalProperty()`
- `jmpSetGrainSizes()`
- `jmpSetTitaniumGrainSizes()`
- `jmpSetGraphiteType()`
- `jmpSetSummaryReadMode()`
- `jmpSetUserFilename()`
- `jmpSetColdfirePhaseReadMode()`
- `jmpSetColdfirePhases()`
- `jmpExcludeColdfirePhases()`
- `jmpGetFoundPhases()`
- `jmpRunColdfireCalculation()`

API documentation : Solidification module

- `jmpSetCastIronType()`
- `jmpSetSolidificationTemperatures()`
- `jmpSetSolidificationPhaseReadMode()`
- `jmpSetSolidificationPhases()`
- `jmpExcludeSolidificationPhases()`
- `jmpRunSolidificationCalculation()`