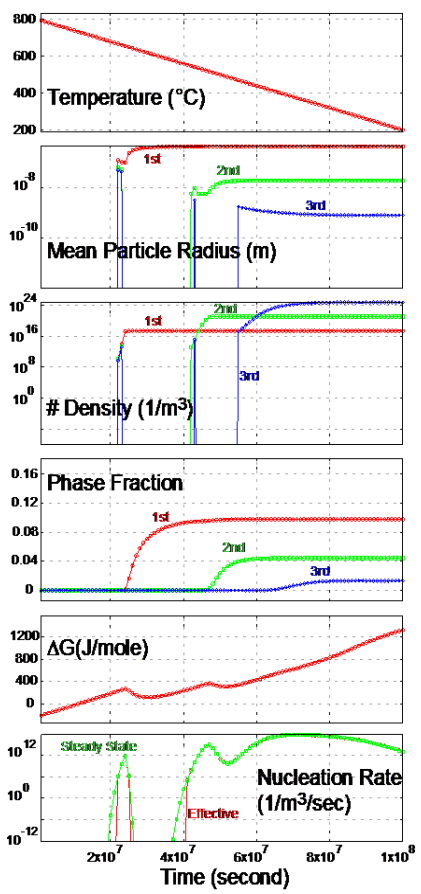
QUESTEK® INNOVATIONS LLC

PrecipiCalc®

PRECIPItation CALCulation for Materials/Process Design and Optimization

Sample *PrecipiCalc* time evolution results of hierarchical precipitation development



General Description

PrecipiCalc is a sophisticated computer program for calculating the 3D multiparticle diffusive precipitation kinetics of multiple phases. Incorporating the Thermo-Calc® Advanced Programming Interface (TCAPI), *PrecipiCalc* adopts multicomponent thermodynamics and mobility, based on the CALPHAD methodology, in its precipitation models. This allows realistic and mechanistic modeling on nucleation, growth and coarsening without resorting to *ad hoc* treatments. The primary input of *PrecipiCalc* software includes:

- Physical quantities such as material compositions, bulk thermodynamics and mobility (TDB files), interfacial properties (such as surface energy and interfacial dissipation) and lattice properties (such as molar volume).
- Thermal cycle, or temperature profile, which defines the thermal history of the material being processed. The thermal cycle can be constant (isothermal), linear cooling (quench) or complicated nonlinear and non-monotonic heat treatments (such as multi-step tempering).

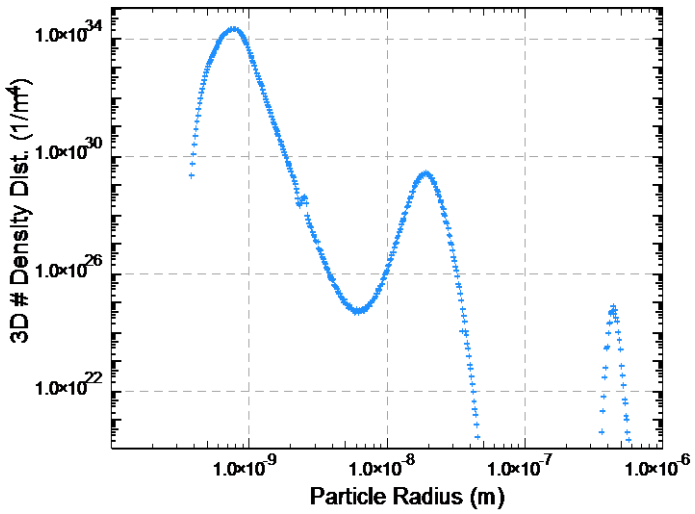
The output of *PrecipiCalc* software includes the time evolution of:

- Precipitate microstructure — precipitate size distribution, number density and volume fraction, which can be used to construct TTT/CCT diagrams.
- Compositions of matrix and precipitate.
- Driving forces, nucleation rates and critical radii.

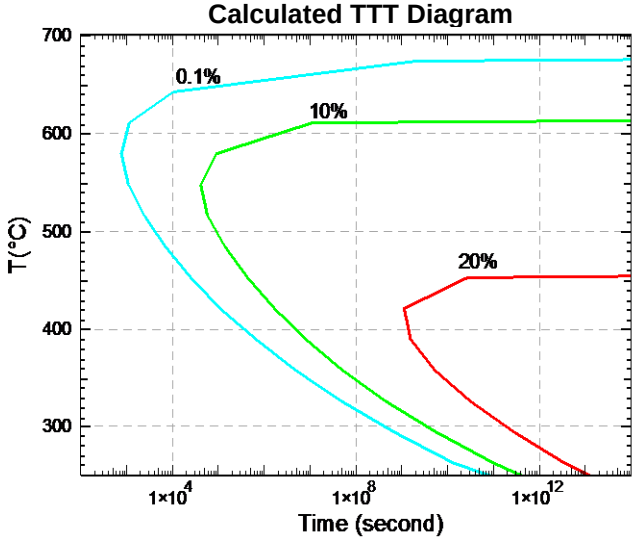
Due to the mechanistic nature of *PrecipiCalc* software, it has been successfully applied to computational material designs and process optimization for a wide range of metallic systems, including

- γ', carbides and borides in Ni-based superalloys.
- Carbide/nitride/intermetallic grain refiners (in weld HAZ) and strengthening dispersions (during tempering) in steels.
- Primary inclusion and strengthening phases in Al-based metals.
- Heusler phase in NiTi-based shape memory alloys.

Calculated Number Density Distribution



Calculated TTT Diagram



* All examples in this page are γ' precipitation in Ni-12at%Al using ThermoTech Ni-Data, NIST mobility database and a fictitious surface energy

For additional information regarding QuesTek's PrecipiCalc contact ***Dr. Jiadong Gong*** *by email at info@questek.com or call 847.425.8221.*

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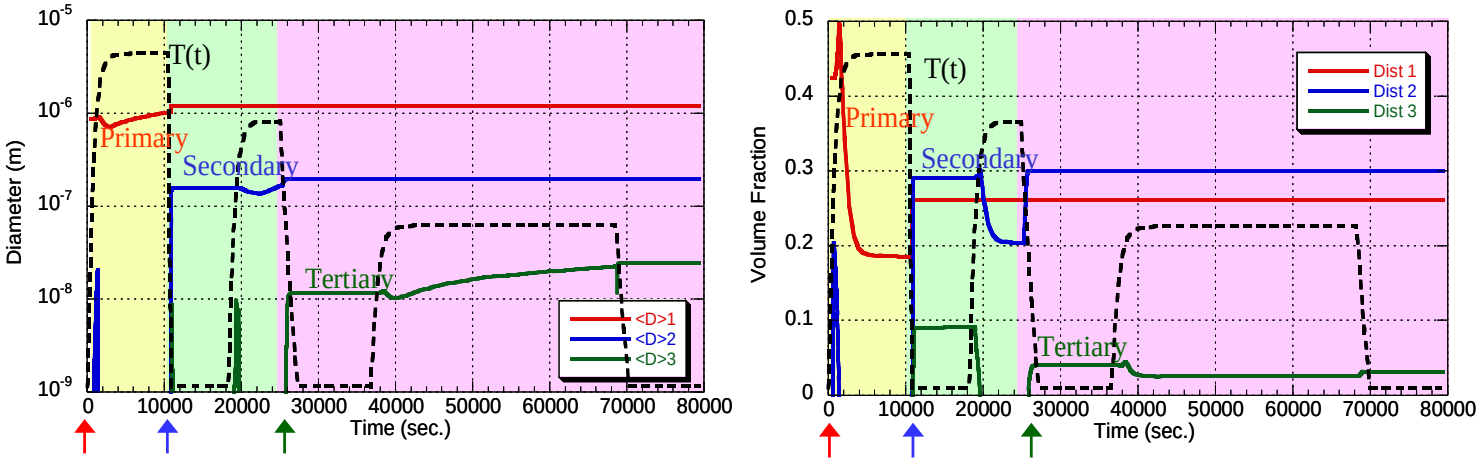
PrecipiCalc

PRECIPItation CALCulation for Materials/Process Design and Optimization

PrecipiCalc Application for an Aeroturbine Disk Alloy

(Work Performed Under DARPA Accelerated Insertion of Materials Initiative)



The above two plots show an example of *PrecipiCalc* γ' precipitation calculation for an aeroturbine disk Ni-based superalloy (IN100) under a complex commercial heat treatment. Three distinct γ' particle size distributions at multiple scale (10nm to 1μm) are observed experimentally and validated in this calculation. Integrating the *PrecipiCalc* calculation with the FEM heat transfer simulation and a strength model, it is possible to capture the spatial microstructure/property variation in the disk and to allow for mechanistic uncertainly analysis, both of which are critical tools in accelerating the material development cycle.

Software Requirements

- Windows XP Professional or Linux on PC/Intel.
- Thermodynamics and mobility databases for TCAPI. They are not provided as part of the *PrecipiCalc* software.
- Freeware Cygwin/XFree86 for Windows and GRACE/PLOTMTV software utilities are recommended to visualize *PrecipiCalc* results.

Availability

Licensing of *PrecipiCalc* software is available for fixed or floating seat arrangement. Discounts are available for academic use and for commercial entities within a material development partnership with QuesTek Innovations LLC.

Technical Description of *PrecipiCalc* Models

PrecipiCalc software solves the following equations numerically:

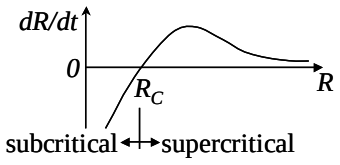
- Continuity equation for the evolution of particle size distribution; no assumption is placed on the form of distribution.
- Homogeneous and heterogenous nucleation with multicomponent effects and a non-isothermal transient/incubation model.
- Mass balance; either perfect or no composition mixing inside particles.
- 3D multiparticle and multicomponent diffusion in matrix based on mean field and steady state assumptions in a sharp interface model. The resulting particle growth rate can be summarized in the equations below. Entire matrices of diffusivity and free energy derivatives are fully utilized in *PrecipiCalc* calculations to capture the multicomponent effects.

$$\text{Growth}: \frac{dR}{dt} = \frac{\left(1 + R\sqrt{4\pi N_v \langle R \rangle}\right)}{\left(R\Gamma + s(R)\Big/\left(M_0 \exp\frac{-Q}{RT}\right)\right)}\left\{\Delta G_m - \frac{2\sigma(R)\bar{V}_m^{\beta}}{R}\right\}$$

$$\text{where } \Delta G_m = \left[\Delta C_i\right]^T \left[\frac{\partial^2 \bar{G}^{\alpha}}{\partial C_i \partial C_j}\right]\left[\Delta C_j^{\infty}\right] + \left[\bar{C}_m^{\beta}\right] \bullet \left(\left[\bar{\mu}_m^{\alpha}\right] - \left[\bar{\mu}_m^{\beta}\right]\right)$$

$$\Gamma = \left[\Delta C_i\right]^T \left[\frac{\partial^2 \bar{G}^{\alpha}}{\partial C_i \partial C_j}\right]\left[D_{jk}\right]^{-1}\left[\Delta C_k^{e}\right]$$

Thermodynamics
Diffusivity
Interfacial Property



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