Square-Root Diffusivity Method
RPI MatLab© Code

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Outline

- Introduction
- Background & Needs
  - *Profiler*, a DOS code (M.K. Stalker, J.E. Morral)
  - *Acta Materialia*, **51**, 1181-1193, 2003 (MEG & AL)
- RPI's MatLab© Multicomponent Diffusion Code
- Testing the code:
  - » 10% Cr –10 %Al –80 %Ni
  - » 43.5% Ni –25 %Zn –31.5 %Cu
  - » 42% Ni –39 %Al – 19% Fe
  - » 32.39% Fe–49.41% Mg–18.20% Ca
- Results

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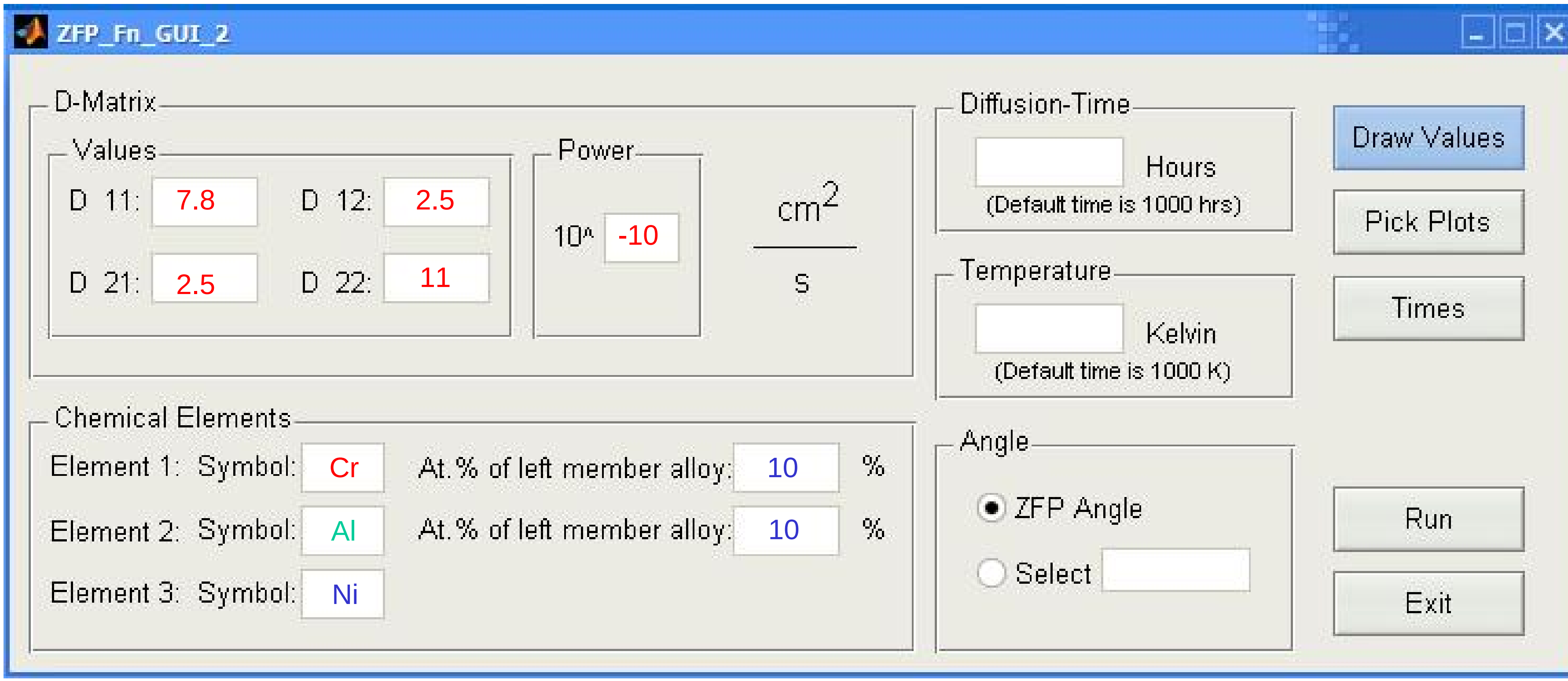
RPI Matlab© Code: GUI



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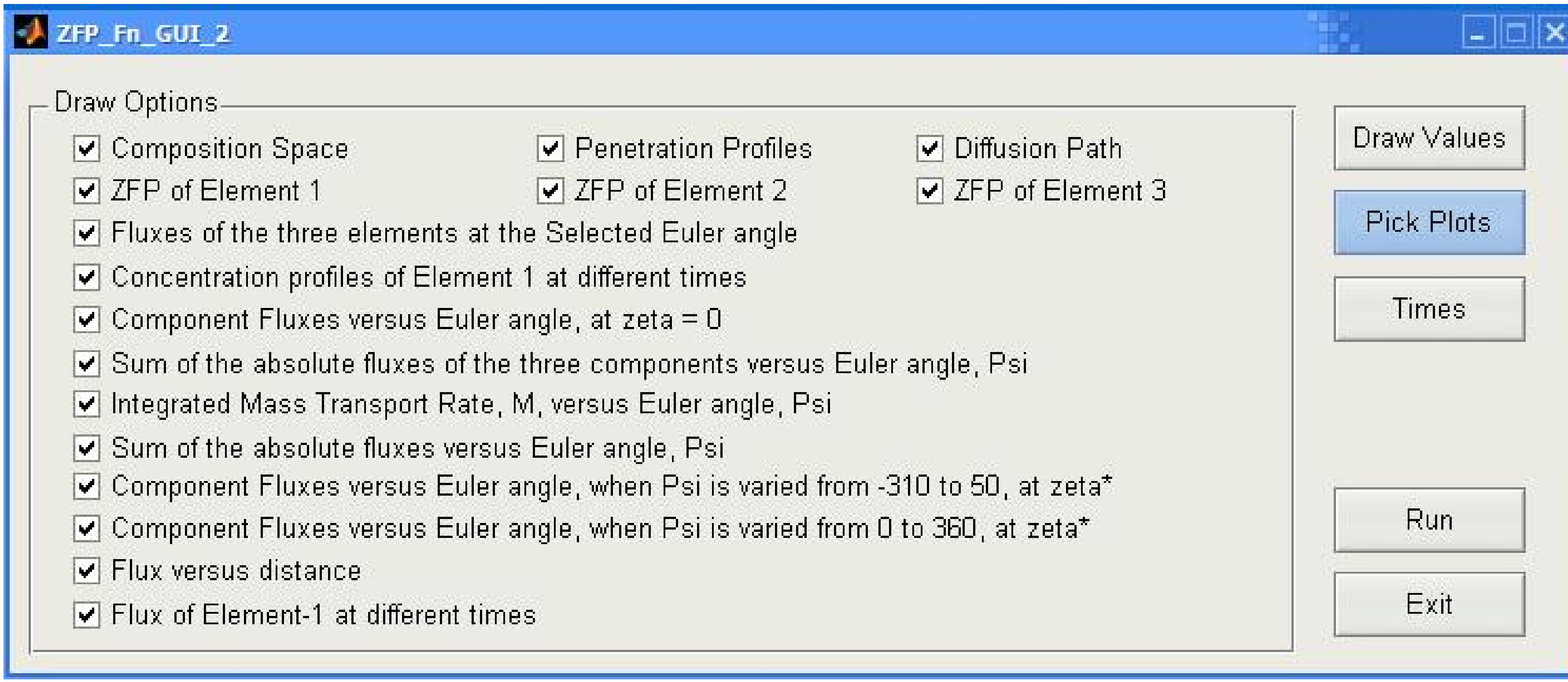
RPI Matlab© Code: GUI



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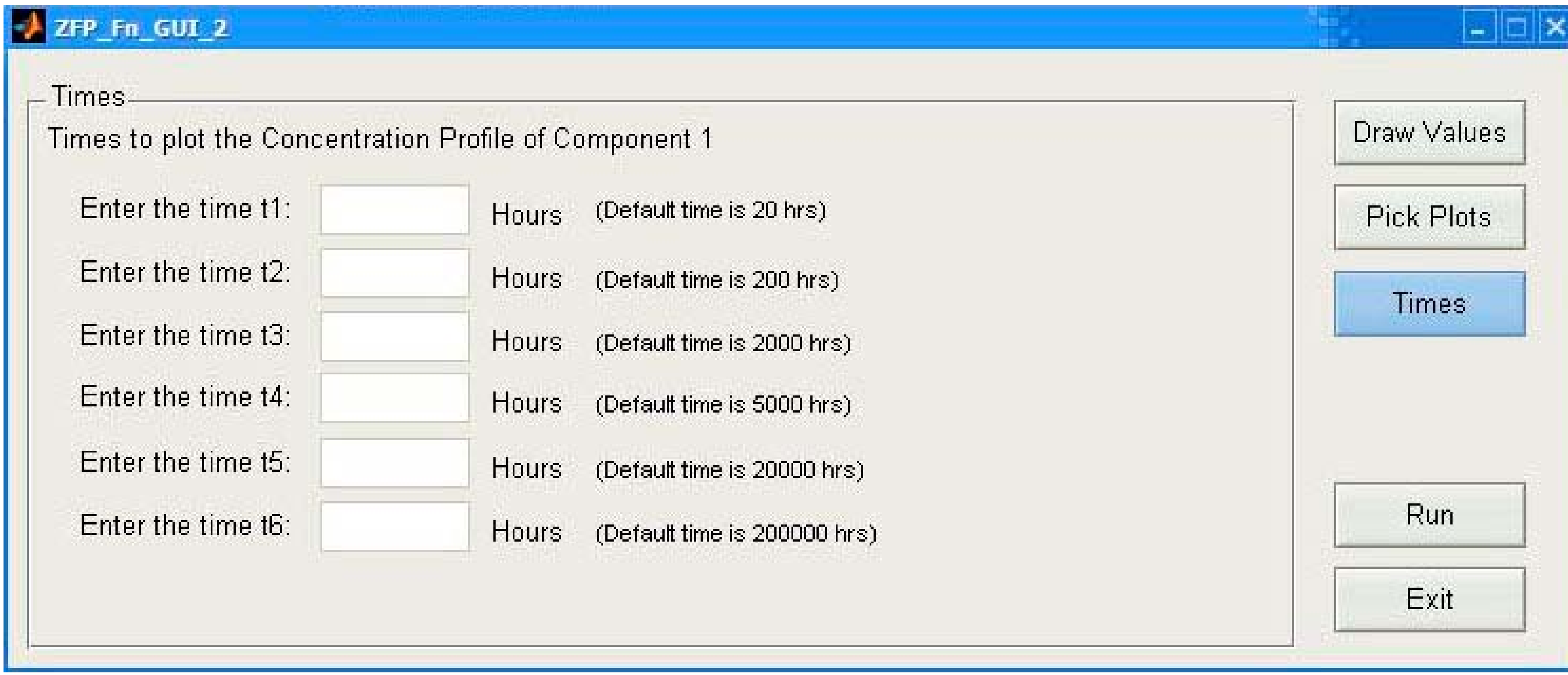
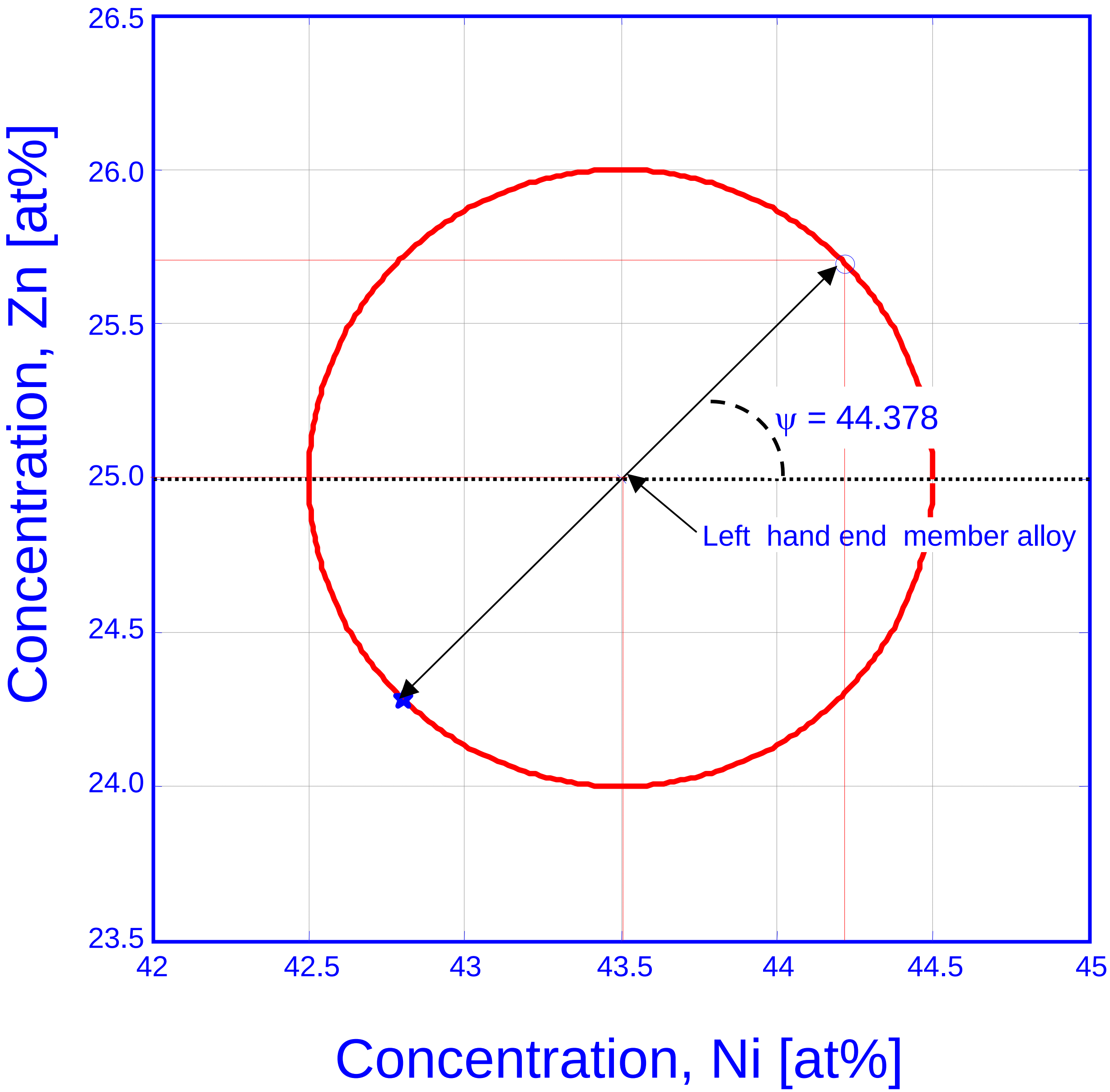
RPI Matlab© Code: GUI



Composition Space



Ni=43.5, Zn=25, Cu=31.5 [at%]

T=1048 K

t= 48 h

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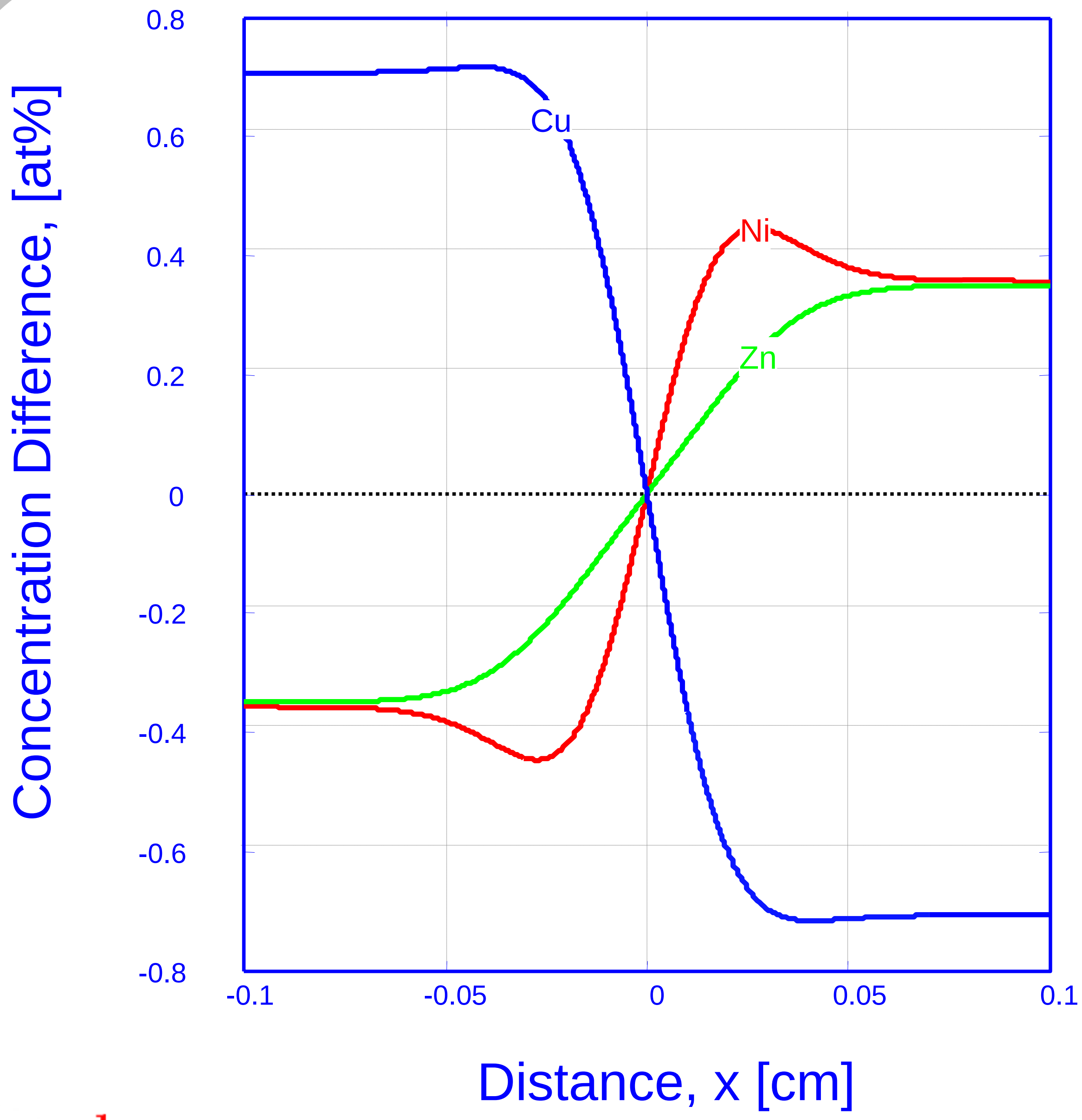
Penetration Profiles



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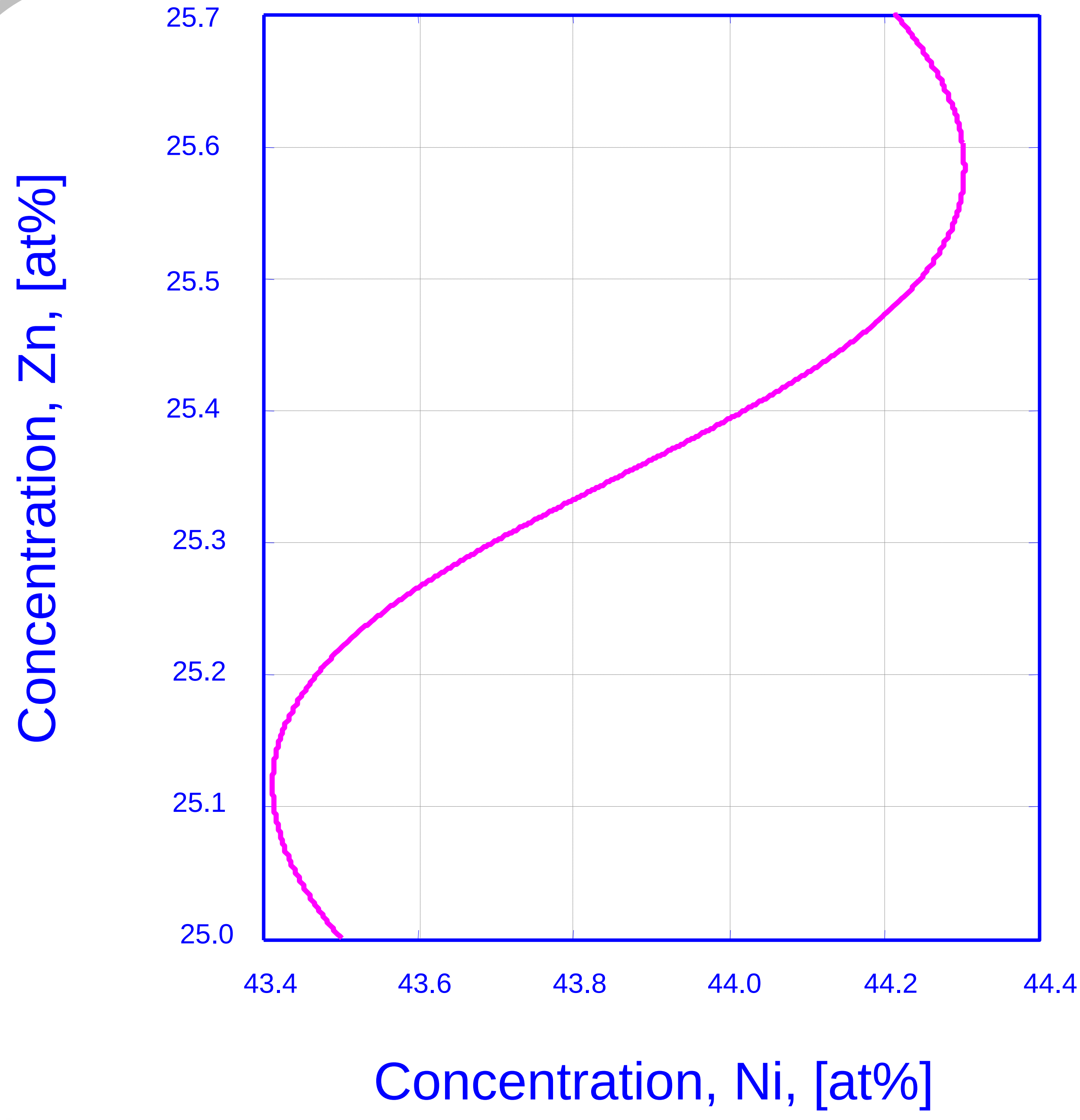

Diffusion Path

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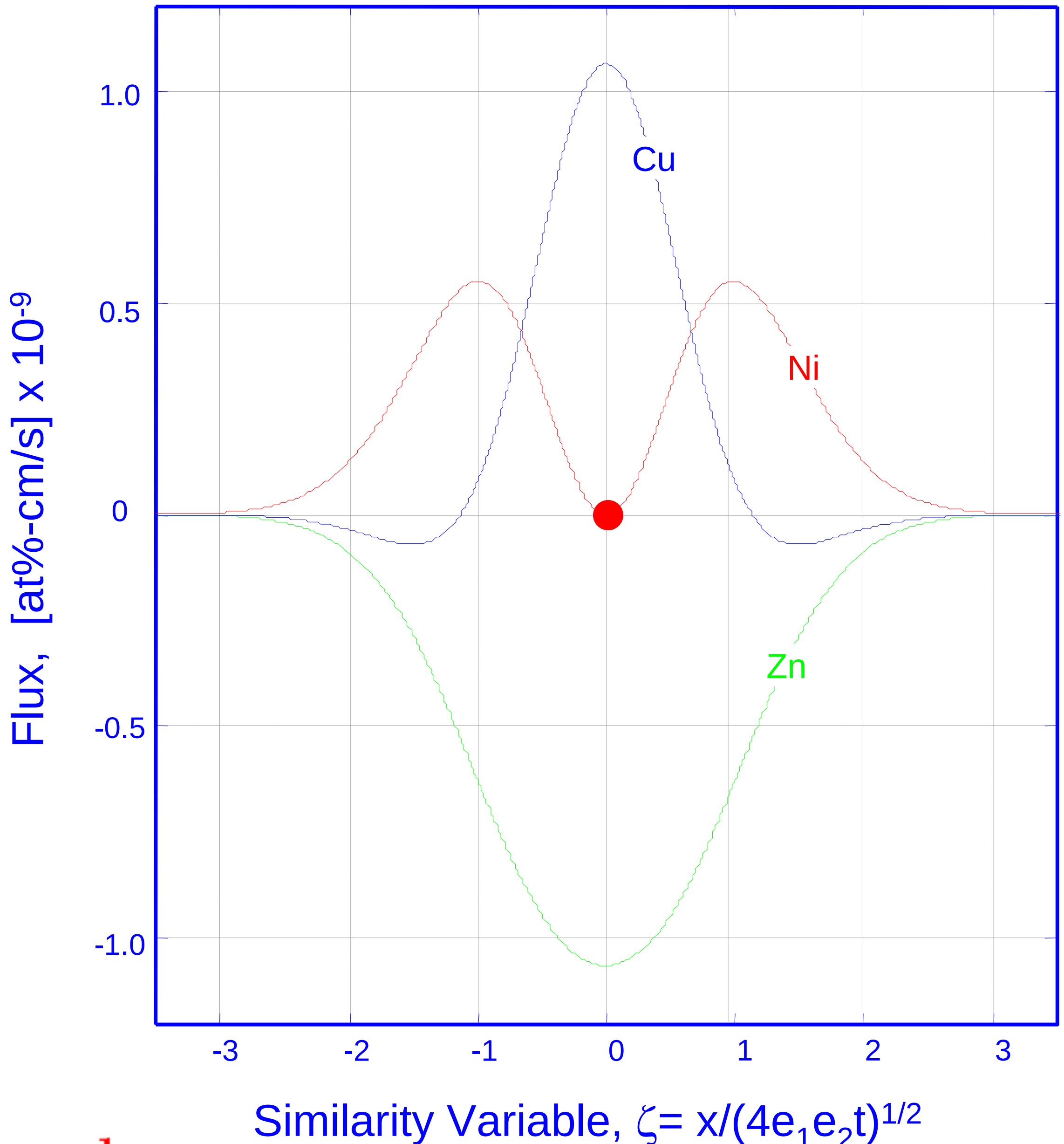
Stationary ZFP for Ni

$\psi = 44.378^\circ$



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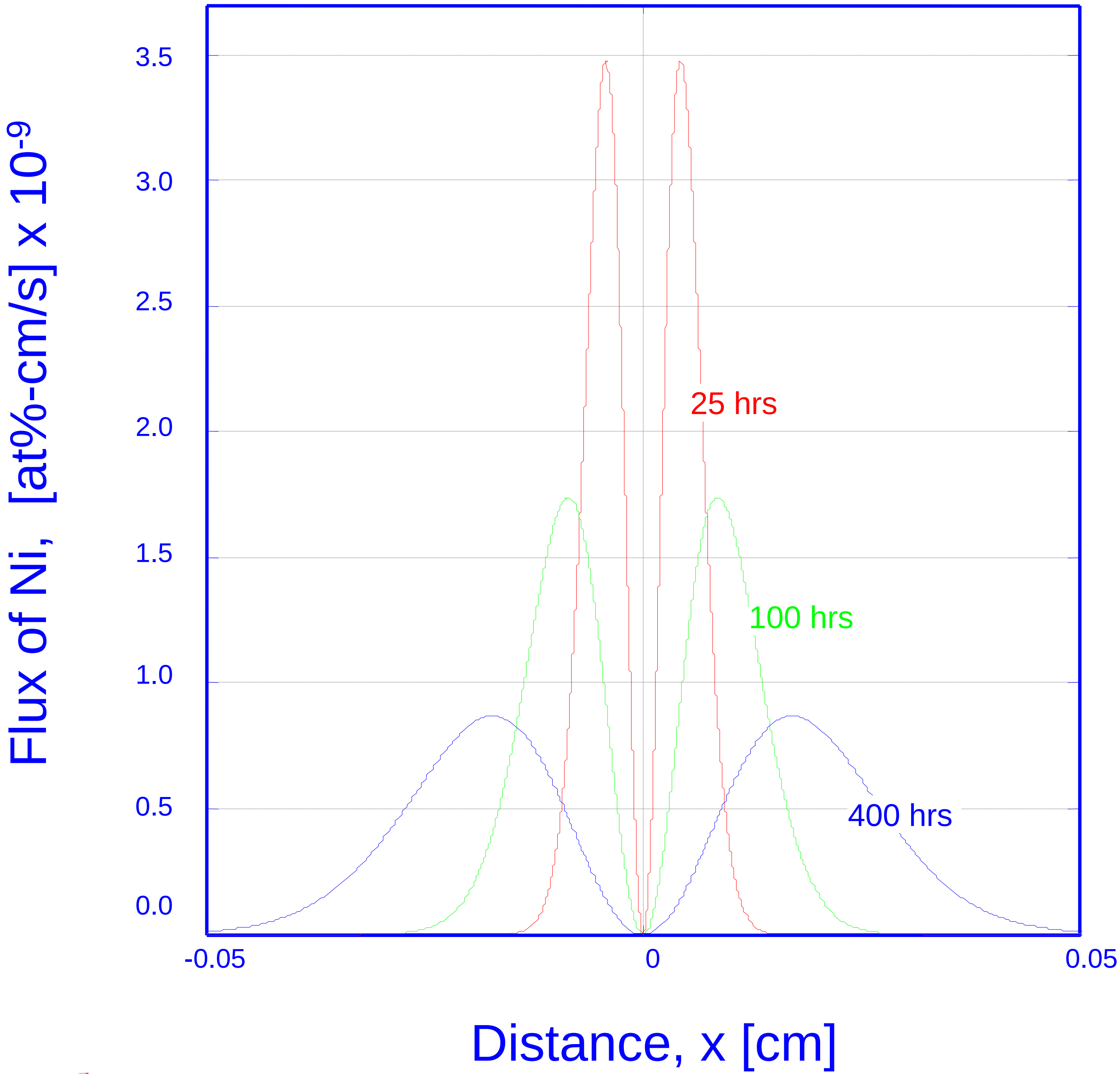
Ni Flux at Different Times



$\psi = 44.378^{\circ}$

$\zeta = 0$

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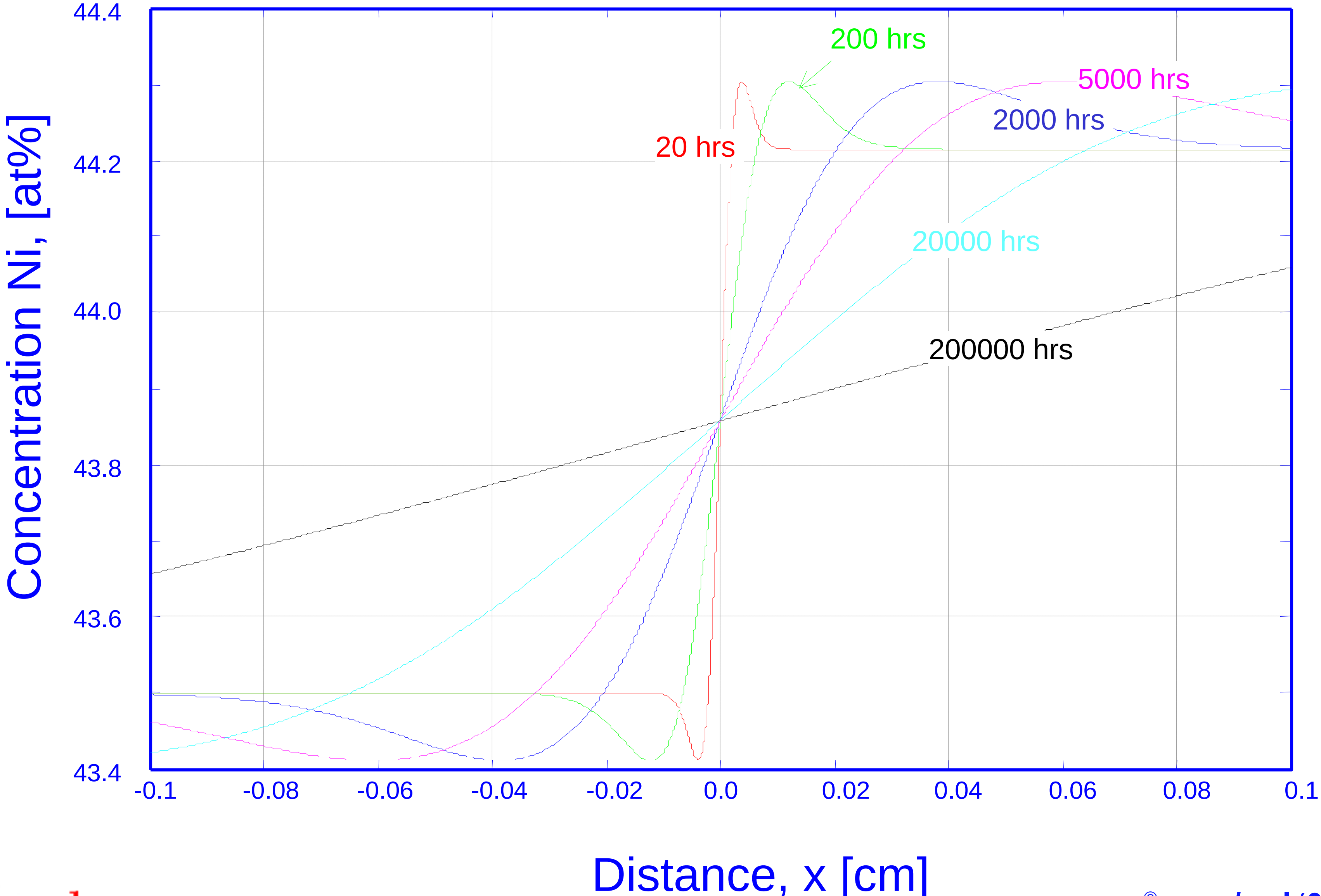
Concentration Profiles for Ni at Different Times



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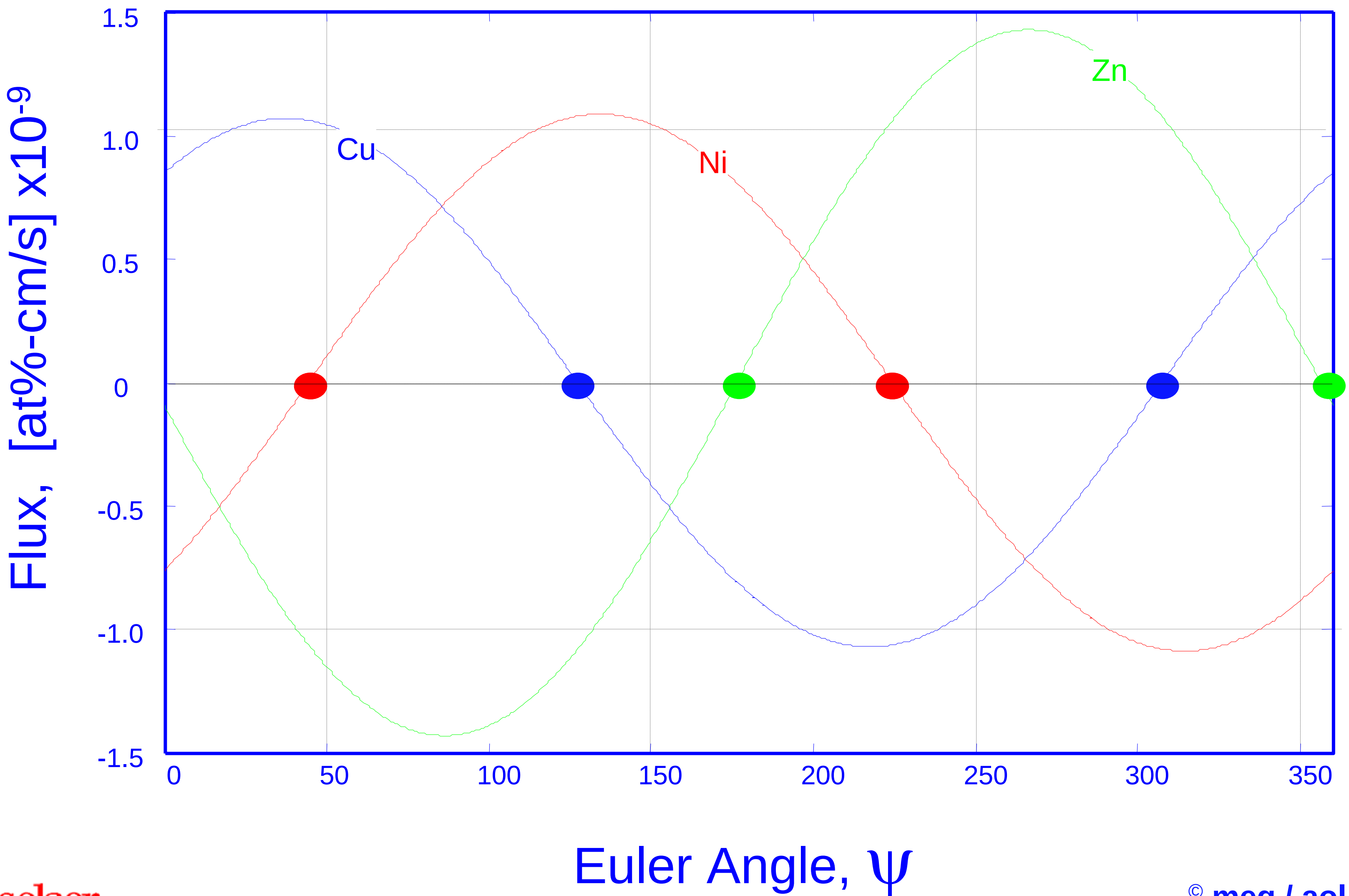
Component Fluxes vs. ψ

$\zeta = 0$



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Integrated Mass Concept

- The absolute transport rate for a ternary diffusion zone

$$M \qquad \overset{3}{\underset{i \;\; 1}{}} \left| J_i \right| \, d$$

- Carrying out the integration

$$M \quad \frac{1}{\sqrt{e_1 e_2 t}} \begin{array}{l} \left| D_{11} \, A_{11} \quad A_{12} \quad D_{12} \, A_{21} \quad A_{22} \right| \quad \left| D_{21} \, A_{11} \quad A_{12} \quad D_{22} \, A_{21} \quad A_{22} \right| \\ \left| D_{11} \quad D_{21} \quad A_{11} \quad A_{12} \quad D_{12} \quad D_{22} \quad A_{21} \quad A_{22} \right| \end{array}$$

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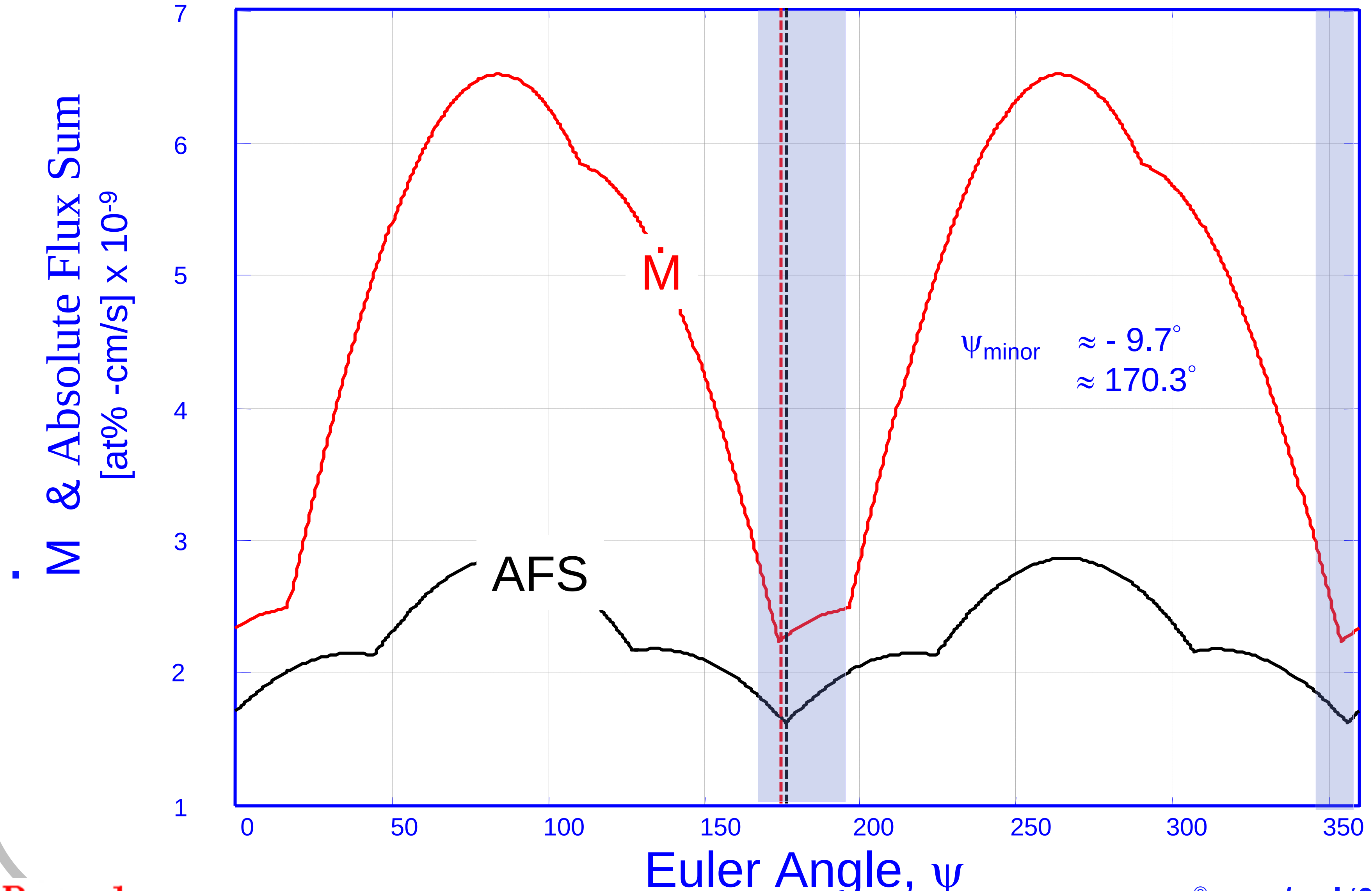
Ni–43.5, Zn–25, Cu–31.5 [at%]



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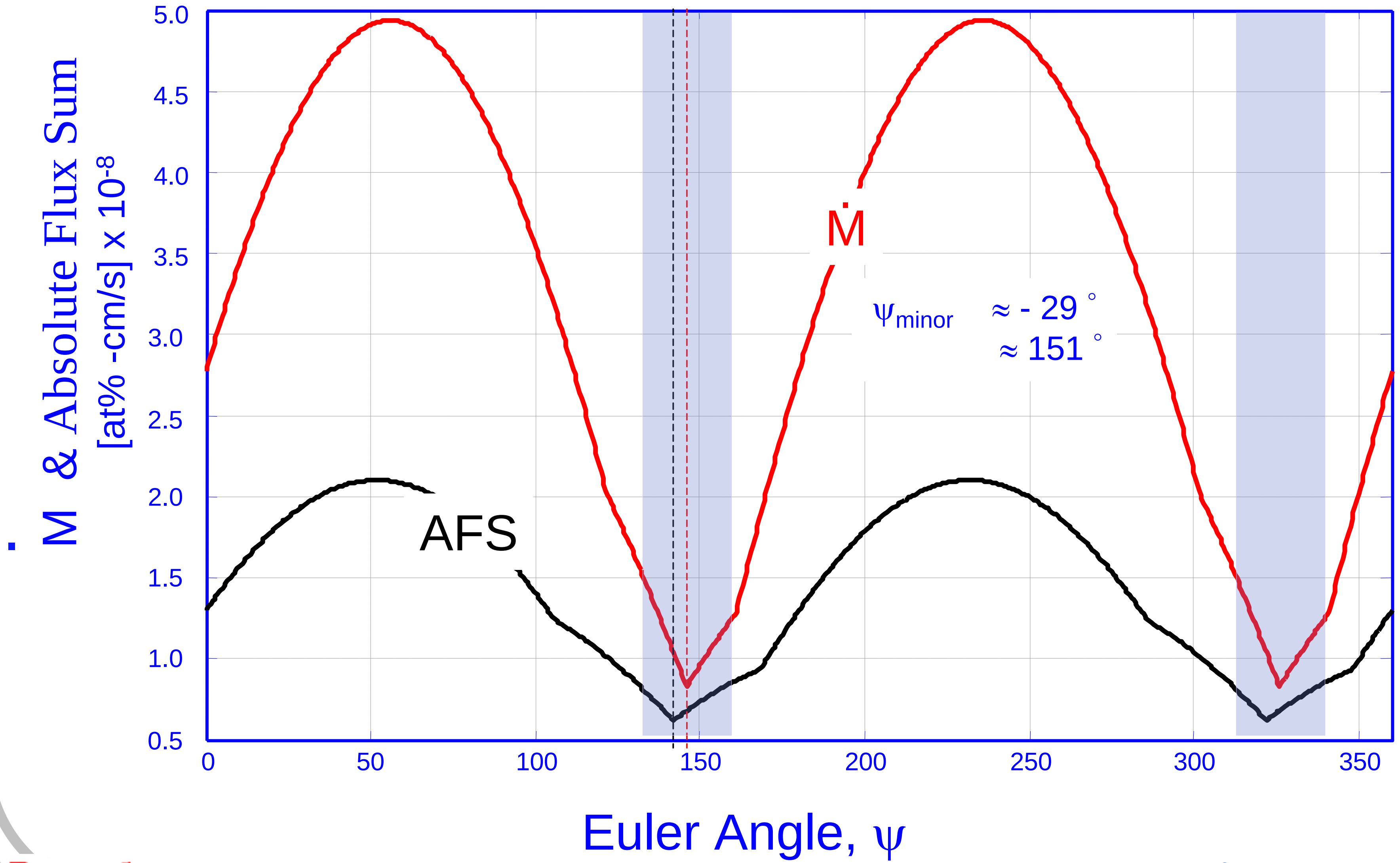
Cr–10, Al–10, Ni–80 [at%]



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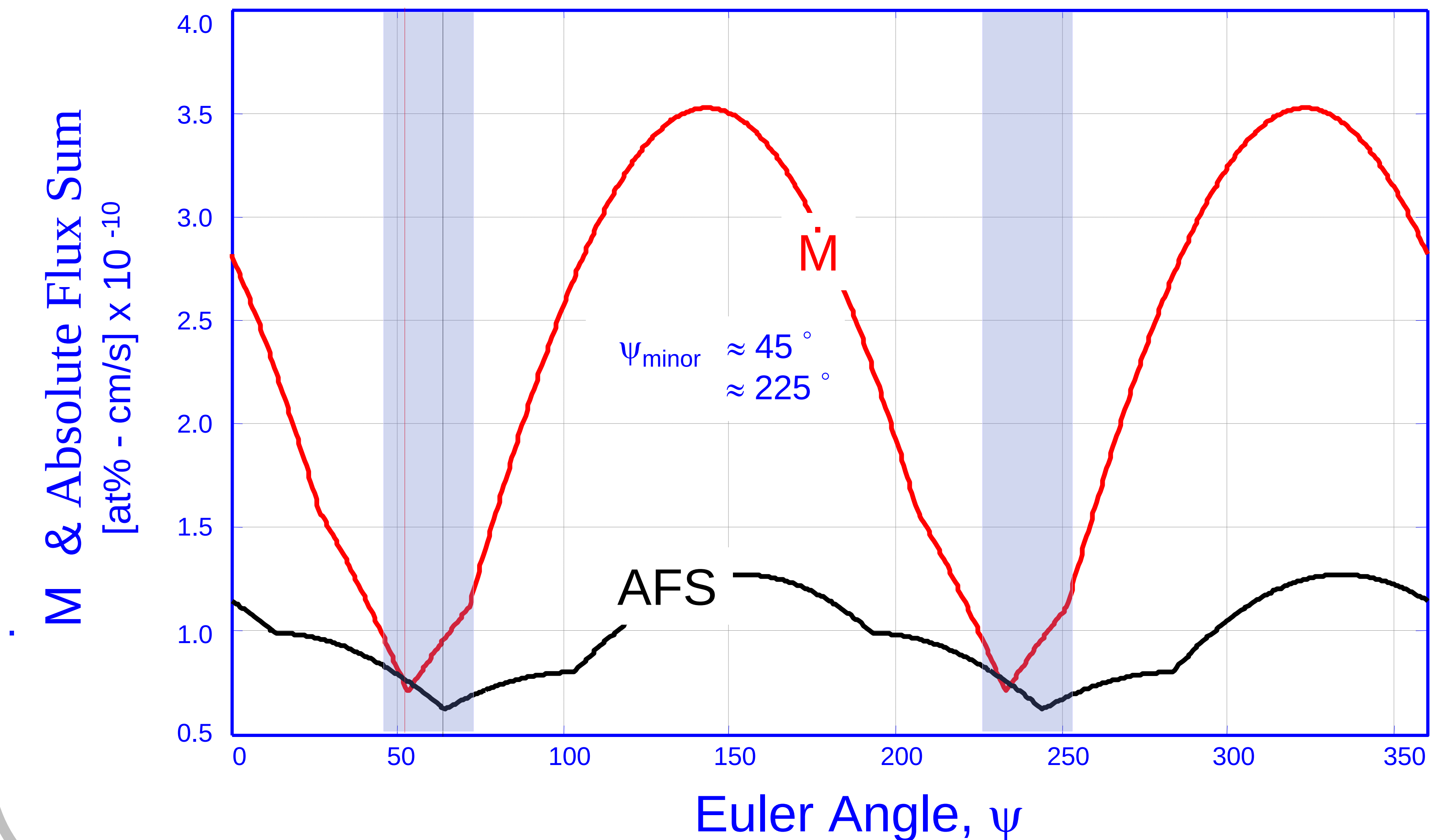
Ni–42, Al–39, Fe–19 [at%]



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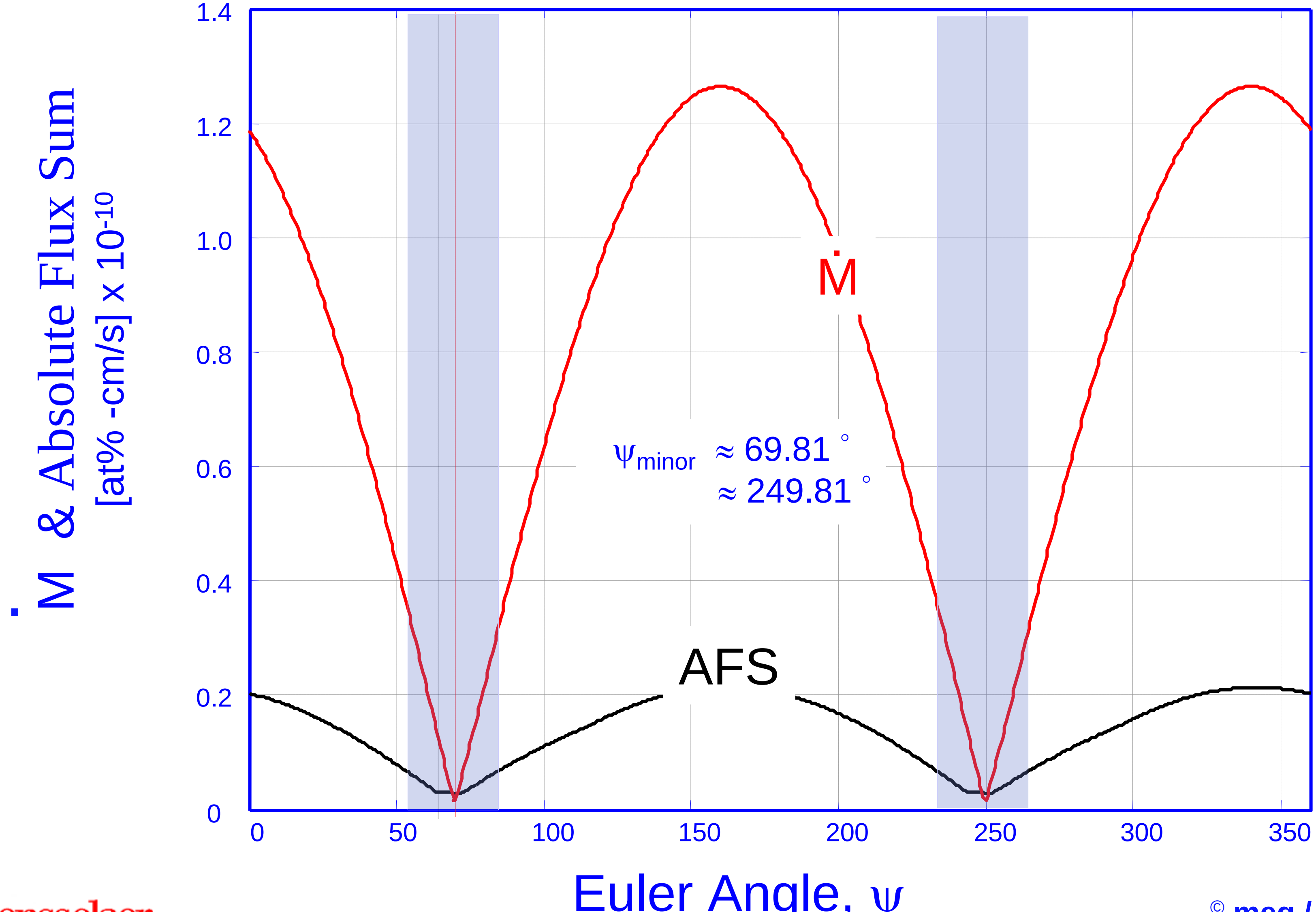
Fe–32.39, Mg–49.41, Ca–18.20 [at%]



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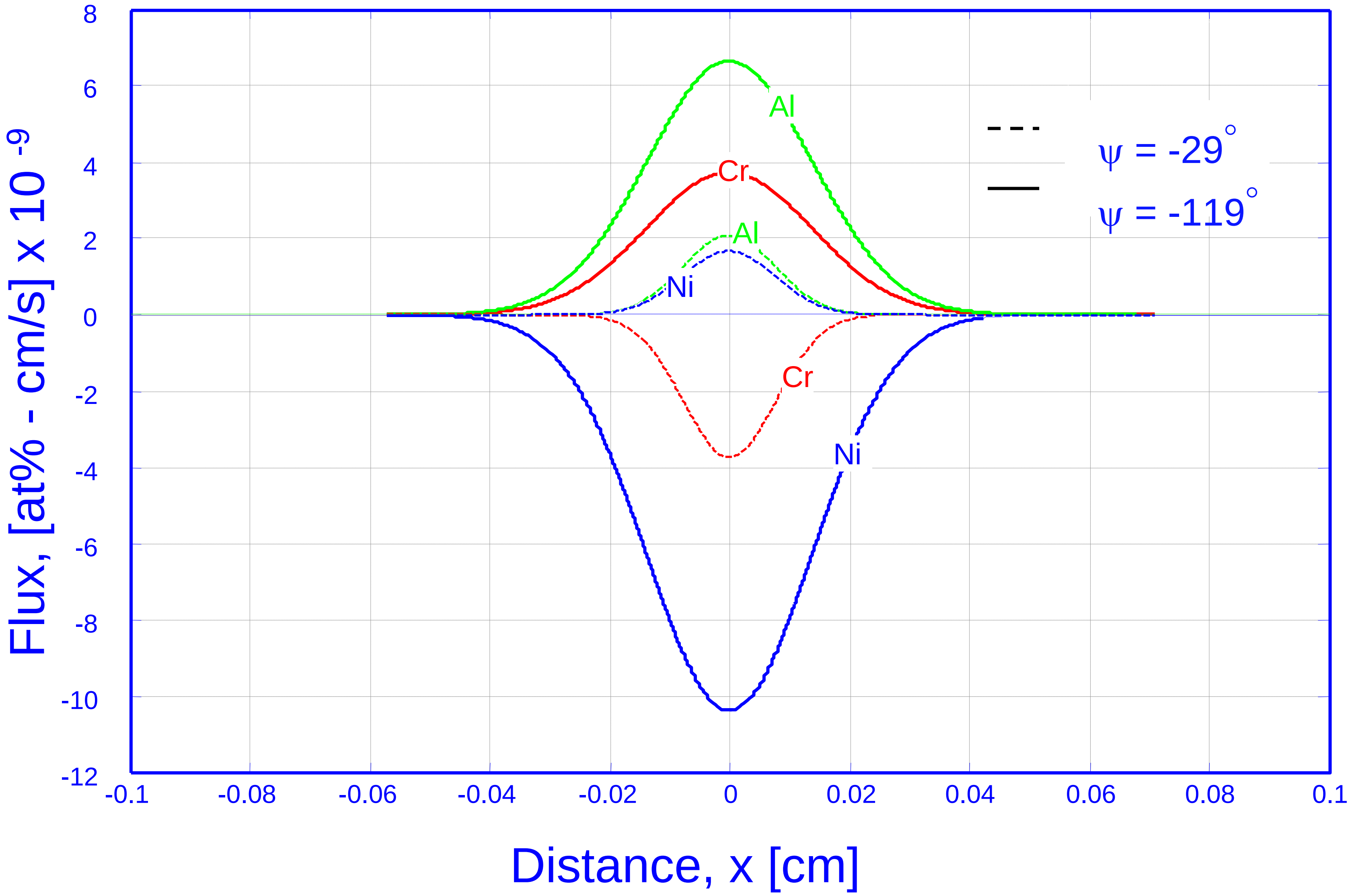
Flux versus Distance



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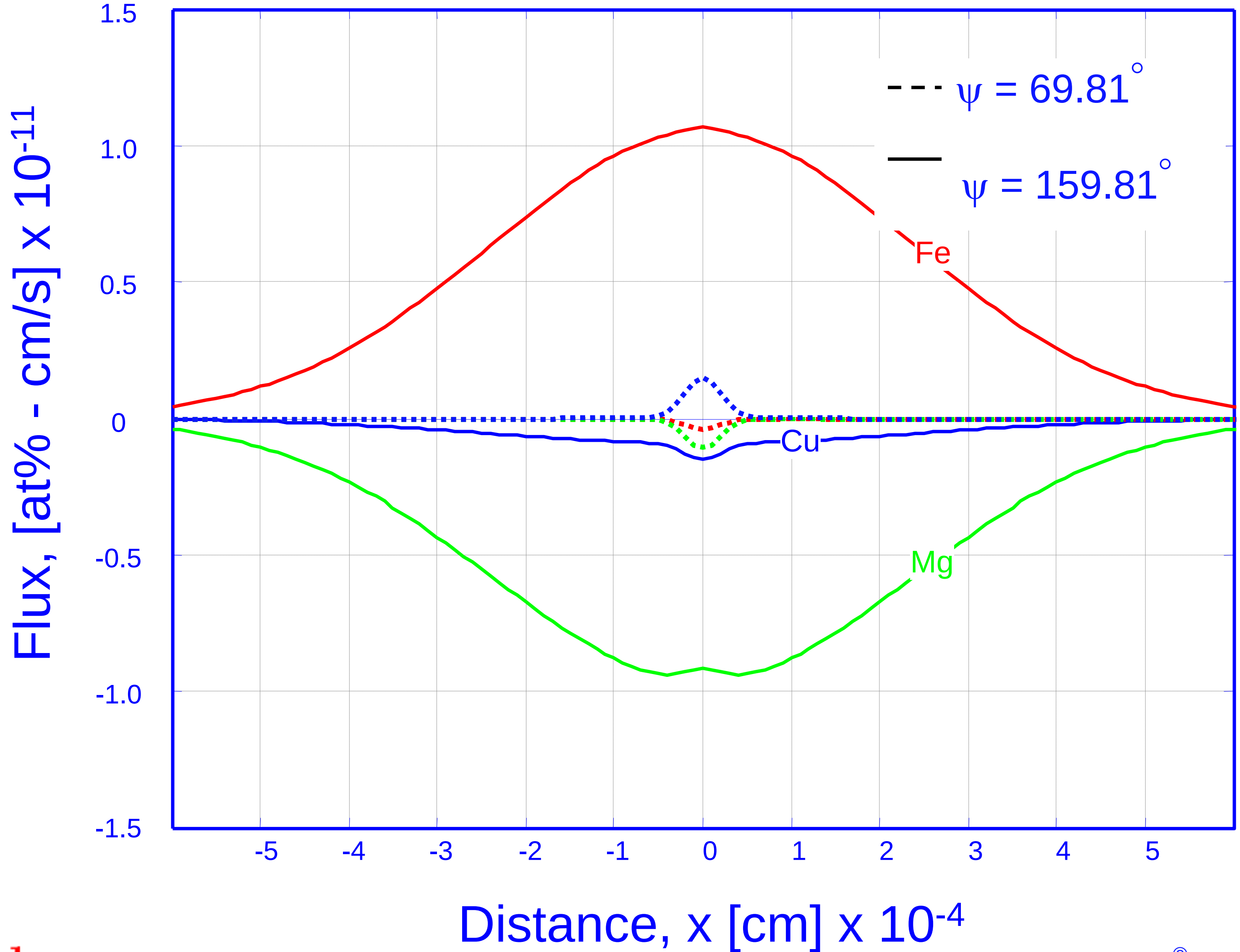
Flux versus Distance



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Composition [at%]	ψ* deg	Minimum M Euler Angle	Minimum Abs. Flux Euler Angle	Stationary ZFP Euler Angle
Cr – 10 Al – 10 Ni – 80	≈ -29 ≈ 151	≈ 145	≈ 140	≈ -38.1 ≈ 141.9 (Ni)
Ni – 42 Al – 39 Fe –19	≈ 45 ≈ 225	≈ 52	≈ 62	≈ 64.31 ≈ 244.31 (Ni)
Ni – 43.50 Zn – 25.00 Cu – 31.50	≈ -9.7 ≈ 170.3	≈ 172	≈ 175	≈ -3.64 ≈176.36 (Zn)
Fe – 32.39 Mg – 49.41 Ca – 18.20	≈ 69.8 ≈ 249.8	≈ 72	≈ 65	≈71.94 ≈ 251.94 (Fe)

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Summary

- A new MatLab code was developed at RPI to simulate multicomponent diffusion in single-phase ternary alloy systems.
- Numerical data obtained using MatLab script was compared with the output provided by *Profiler* (DOS), and *Kaleidagraph*© (Mac-OS).
- The new code was tested with a few alloy sytems including the ternary alloy, 43.5 at%-Ni, 25 at%-Zn, 31.5 at%-Cu, where diffusive spreading is reduced for couples located in composition space close to the minor eigenvalues located at $\psi^*= -9.65^o$ and $\psi^*=170.34^o$.
- Stationary ZFPs of the minor component occur at $\psi^{Zn}_{ZFP}= -3.64^o$ and also$\psi^{Zn}_{ZFP}= 176.36^o$.
- We predict the end-member compositions for which minimum mass transport rate, *M*, occurs and for different systems.
- Code development work remains in progress.

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