Assignment#4
Computational Material Thermodynamics

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Using Muggianu, Colinet and Kohler extrapolation methods and limiting binary models (refer Table 1), plot the $\triangle_{mix}H_m$ for $Ni_{10}T_{30}V_{60-y}Zr_y$ $\forall$ $y = 0$ to 60.

System	$\triangle_{mix}H_m$
Nb-Ti	$x_{Nb}x_{Ti}(+3000)$
Nb-V	$x_{Nb}x_V(-1875)$
Nb-Zr	$x_{Nb}x_{Zr}(-10311 + 6709(x_{Nb} - x_{Zr}))$
Ti-V	$x_{Ti}x_V(7600 + 2200(x_{Ti} - x_V))$
Ti-Zr	$x_{Ti}x_{Zr}(-968)$
V-Zr	$x_V x_{Zr}(-14900 + 3000x_{Zr} + 1000x_{Zr}^2)$

Table 1: Binary Data

In Figure 1, Muggianu and Colinet extrapolation curves almost overlap while Kohler extrapolation curve is separate.

$\triangle_{mix}H_m$ for equiatomic quaternary alloy: $Ni_{25}Ti_{25}V_{25}Zr_{25}$ is shown in Table 2.

Method	Value
Muggianu	-981.5000
Kohler	-981.5000
Colinet	-977.5938

Table 2: Equiatomic Quaternary Alloy

MATLAB scripts for all six binary models and three extrapolation methods were written and can be found in the same folder as this report. Execute *extrapolate.m* to generate the reported plots and data.
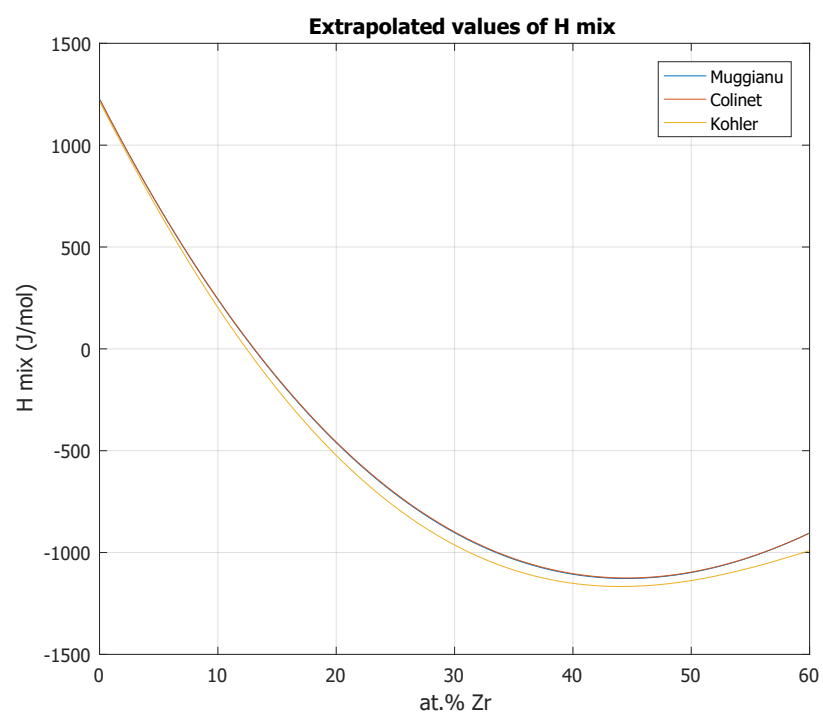
Figure 1: Combined plot of all three extrapolation methods