We use the following expression to compute heat flux for Ar-Cu nanofluids:

$$J_Q = \sum_{\alpha=1}^{2}\sum_{j=1}^{N_\alpha}\frac{1}{2}m_\alpha v^2{}_{j\alpha}\mathbf{v}_{j\alpha} - \frac{1}{2}\sum_{\alpha=1}^{2}\sum_{\beta=1}^{2}\sum_{j=1}^{N_\alpha}\sum_{\substack{k=1\\k\neq j}}^{N_\beta}\left[r_{j\alpha k\beta}\frac{\partial\phi(r_{j\alpha k\beta})}{\partial r_{j\alpha k\beta}} - \phi(r_{j\alpha k\beta})\mathbf{I}\right]\mathbf{v}_{j\alpha} - \sum_{\alpha=1}^{2}h_\alpha\sum_{j=1}^{N_\alpha}\mathbf{v}_{j\alpha}$$

Now there are two methods of partial enthalpy calculation for Ar and Cu, please check it for me if one of it is right or both is wrong, thanks so much

1. According to "We calculated the average enthalpy as the sum of the average kinetic energy, potential energy and average virial terms per particle of each species." in Sarkar's "Thermal Conductivity Computation of Nanofluids by Equilibrium Molecular Dynamics Simulation: Nanoparticle Loading and Temperature Effect", we compute partial enthalpy for Ar and Cu as

$$h_{Ar} = \frac{1}{N_{Ar}}\sum_{i=1}^{N_{Ar}}\left(ke_i + pe_i + \vec{r}_i\cdot\vec{f}_i\right)$$

$$h_{Cu} = \frac{1}{N_{Cu}}\sum_{i=1}^{N_{Cu}}\left(ke_i + pe_i + \vec{r}_i\cdot\vec{f}_i\right)$$

2. According to the expression within Hoheisel's article "Thermal transport coefficients for one-and two-component liquids from time correlation functions computed by molecular dynamics":

One may, however, approximately 'share' the total enthalpy between the components and define a molecular formulation of the partial enthalpy on this route. Using that approximation for h_1 (in analogy with the total enthalpy), we find:

$$h_1 = \tfrac{5}{2} k_B T - \frac{1}{6N} \sum_{\alpha=1}^{2} \sum_{i \neq j}^{N_1, N_\alpha} \left(r_{ij}^{(1\alpha)} \nabla \phi\left(r_{ij}^{(1\alpha)}\right) - \phi\left(r_{ij}^{(1\alpha)}\right) \right) \tag{34}$$

with

$$h_2 = h - h_1, \tag{34a}$$

where h denotes the total enthalpy per particle. Using eq. (34a) the third term of the right hand side of eq. (32) may be written:

$$\sum_{\alpha=1}^{2} h_\alpha \sum_{i=1}^{N_\alpha} v_i^{(\alpha)} = \left[\left(1 + \frac{m_1}{m_2}\right) h_1 - \frac{m_1}{m_2} h \right] \sum_{i=1}^{N} v_i^{(1)}. \tag{35}$$

I got partial enthalpy for Ar and Cu as

$$h_{Ar} = \frac{5}{3N} \sum_{i=1}^{N} ke_i + \frac{1}{3N} \sum_{i=1}^{N_{Ar}} \left(pe_i + \vec{r}_i \cdot \vec{f}_i \right)$$

$$h_{Cu} = \frac{5}{3N} \sum_{i=1}^{N} ke_i + \frac{1}{3N} \sum_{i=1}^{N_{Cu}} \left(pe_i + \vec{r}_i \cdot \vec{f}_i \right)$$

$$Where \quad N = N_{Ar} + N_{Cu}$$