Problem 2: constant pressure adiabatic stirred batch reactor with variable heat capacities

The following elementary gas-phase reaction is conducted in a laboratory scale stirred batch reactor:

$$A(g) + B(g) \rightarrow 2C(g) + D(g)$$

The reactor is initially charged with an equimolar mixture of gases A and B, together with other inert species (I). The amount of A introduced is 4 mol and the total amount of gas mixture fed into the reactor is 500 g. The average molecular weight of the feed mixture is 40 g/mol. The gas mixture is at initial temperature of 200 ºC and at pressure of 1 atm. The reactor operates at constant pressure under adiabatic conditions. The reaction is exothermic and the enthalpy change of reaction is -12500 J/(mol C) for a reference temperature of 20 º C. The reaction rate constant is represented by the following expression:

$$ln\ k = 8.2\text{-}1000/T$$ (T is in Kelvin and k y *k* in L·mol^{-1}·h^{-1}).

Calculate the reaction time needed to reach a fractional conversion of 90% for the following cases:

a) Assume an average heat capacity, $Cp_{m,j}$, for each component.

b) Consider the variation of the heat capacity with the temperature for each component according to the following expression:

$$Cp_j(T) = a_j + b_j T + c_j T^2 + d_j T^3\ ,$$ *T* is in degree Celsius

Data:

Component	a_j	$b_j \times 10^2$	$c_j \times 10^5$	$d_j \times 10^9$	$Cp_{m,j}$ (J·mol^{-1}·K^{-1}) (450 K < T <800 K)
A	9.8564	0.0026	0.1124	-0.2973	10
B	11.3934	1.3356	-0.9109	2.3550	15
C	11.5188	0.9680	0.1449	-2.1910	15
D	11.4532	0.0868	0.2260	-1.1339	12
I	10.3337	3.4313	-0.9913	4.8166	20