```
using DifferentialEquations   , Plots
```

# Problem 12-15

```
# physical data
begin
    Eₐ = 4e4 # cal/mol
    R = 1.987 # cal/mol/K
    k⁰ = 6.6e-3 # 1/min
    Fₐ₀ = 80. # mol/min
    cₚ = 50 # cal/mol
    ΔH = -7500. # cal/mol
    Uₐ = 8e3 # cal/min/K
    Tₐ = 300 # K
    τ = 100 # min
end;
```

## (a)

Heat generation:

$$G = r_A \Delta H$$

Heat removal:

$$R = U_A(T_a - T)$$

Rate law:

$$-r_A = kC_{A0}(1 - X_A)$$

$$k = k^0 \exp\left[\frac{-E_a}{R}\left(\frac{1}{T^0} - \frac{1}{T}\right)\right]$$

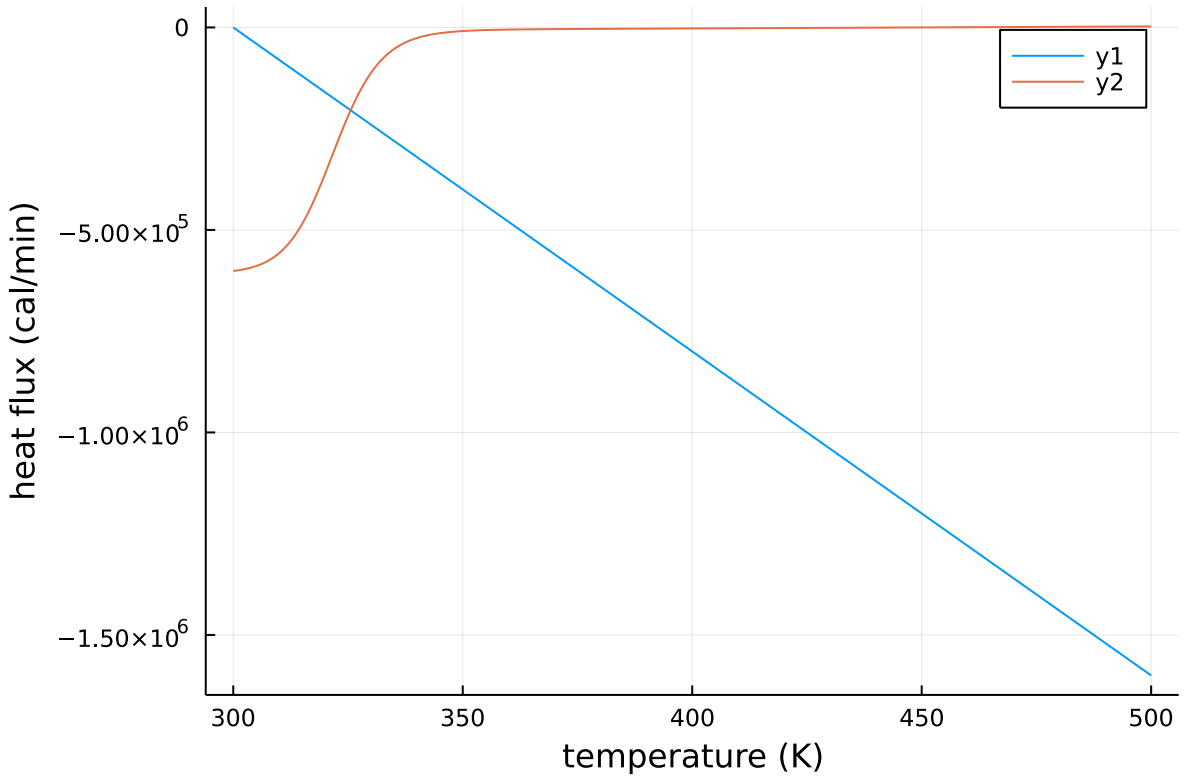
Performance equation:

$$k\tau = \frac{X_A}{1 - X_A}$$

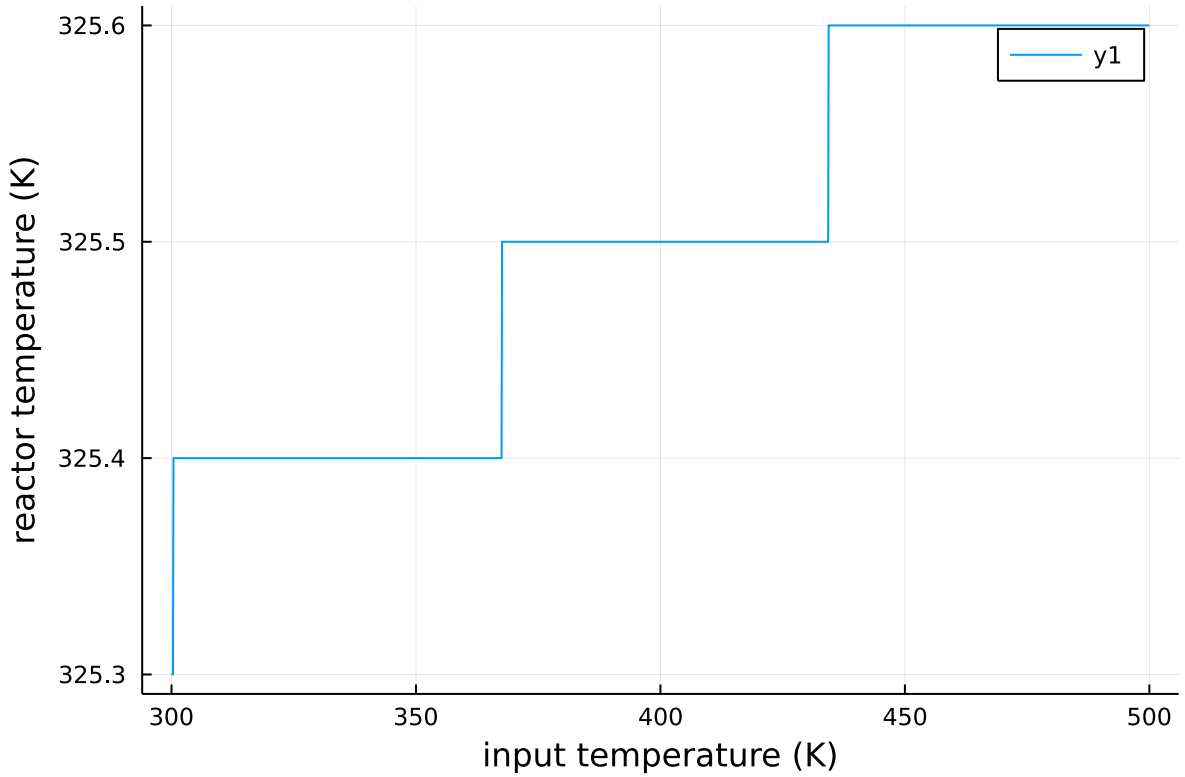
```
begin
    T = [300:0.1:500...]

    r_a(T) = k(T) * F_a0 * (1 - X(T))
    X(T) = k(T) / (1 + k(T))
    k(T) = k⁰ * exp(-E_a * (1/350 - 1/T) / R)

    heat_inp(T; T_0) = c_p * (T - T_0)
    heat_rem(T) = U_a * (T_a - T)
    heat_gen(T) = r_a(T) * ΔH
end;
```

The curves intersect at 326 K, corresponding to 33 % conversion.

```
begin
    Rs = heat_rem.(T)
    Gs = heat_gen.(T) + heat_inp.(T, T_0=450.)
    local i = argmin(abs.(Rs .- Gs))
    local t = Int(round(T[i]))
    local c = Int(round(X(T[i]) * 100))
    md"The curves intersect at $t K, corresponding to $c % conversion."
end
```




**(b)**




```
begin
    function find_T(T₀)
        Rs = heat_rem.(T)
        Gs = heat_gen.(T) + heat_inp.(T, T₀=T₀)
        i = argmin(abs.(Rs .- Gs))
        return T[i]
    end

    plot(T, find_T.(T), xlabel="input temperature (K)", ylabel="reactor temperature (K)")
end
```