

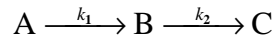
See an example of a **Fortran** 90 program to solve a problem in Chemical Engineering from Robinson [1975, ch. VII, "Chemical Reactor Simulation", p 133, "Thermal Effects"]. Essentially, the application permits understanding some of the features of the Fortran language, the nature of the problem being not relevant.

In the example, only one (the optimal) temperature, $T = 340$ K, will be used, although to find the optimum a temperature range should have to be investigated.

Thermal Effects

(...)

Let us consider the isothermal operation of a tubular reactor in which the reaction



is proceeding. We shall assume constants and initial concentrations as in Table 7.2; these constants have been used elsewhere [Bilous *et al.*, 1956]. We shall simulate the

TABLE 7.2

Tubular reactor conditions	
$k_1 =$	$k_{1,\text{inf}} \exp \frac{-E_1}{RT}$
$k_2 =$	$k_{2,\text{inf}} \exp \frac{-E_2}{RT}$
$k_{1,\text{inf}} =$	$0.535\text{E}+11 \text{ min}^{-1}$
$k_{2,\text{inf}} =$	$0.461\text{E}+18 \text{ min}^{-1}$
$E_1 =$	$18\,000 \text{ kcal/kmol}$
$E_2 =$	$30\,000 \text{ kcal/kmol}$
$R =$	2.0 kcal/kmol-K
At $t = 0,$	
$a_0 =$	0.95 mol/litre
$b_0 =$	0.05 mol/litre

process for which the equations are:

$$\begin{aligned} \frac{da}{dt} &= -k_1 a \\ \frac{db}{dt} &= k_1 a - k_2 b \\ \frac{dc}{dt} &= k_2 b \end{aligned}$$

It will be assumed that B is the desired product; we shall calculate its yield after a reaction time of 10 min, investigating this yield as a function of temperature.

This is carried out in programme 7.3 (...). The yield of B is greatly influenced by the temperature, and an optimal value may be calculated which maximises the yield. (...)

References

- ROBINSON, E. R., 1975, "Time Dependent Chemical Processes", Applied Science Publishers, Ltd., London
- BILOUS, O., and N. AMUNDSON, 1956, "Optimum temperature gradients in tubular reactors", *Chemical Engineering Science*, **5**, 81 and **5**, 115.