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

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

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
$k_1 =$	$k_{1,\inf} \exp \frac{-E_1}{RT}$
$k_2 =$	$k_{2,\inf} \exp \frac{-E_2}{RT}$
$k_{1,\inf} =$	0.535E+11 min^{-1}
$k_{2,\inf} =$	0.461E+18 min^{-1}
$E_1 =$	18 000 kcal / kmol
$E_2 =$	30 000 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:

$$\frac{\mathrm{d}a}{\mathrm{d}t} = -k_1 a$$

$$\frac{\mathrm{d}b}{\mathrm{d}t} = k_1 a - k_2 b$$

$$\frac{\mathrm{d}c}{\mathrm{d}t} = k_2 b$$

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.