Example l0: Catalyst Activity Decay

Example 10 requires the input and program in Example 7. That example file is referenced below.

Reference:C:\Users\Harvey\OneDrive\documents\ebook single phase\Mathcad version - 3\Example 7.xmcd

This example simulates the decline in catalyst activity that results from the sintering of the catalyst above a critical temperature, T_s. The *Rxt2D* program in Example 7 above is used repeatedly to obtain the catalyst temperature profile. A simple decay function has been assumed below. The time constant for the decay process, k_d , and T_s were arbitrarily chosen for demonstration.

$$k_d := \frac{0.5}{hr}$$

$$T_s := 550 \cdot K$$

$$decay(y, t, T_s, k_d) := -k_d \cdot y \cdot \Phi(t - T_s)$$

Decay is assumed first order in activity, y, when the temperature, t, is above T_s. The Heaviside step function, Φ, turns the decay process on and off based on the temperature.

$Age\left(act\ ,NT\ ,tf\ ,T_s\ ,k_d\ ,NZ\right)$:=

"time step size, h"

$h \leftarrow \frac{tf}{NT}$

"initial activity"

for $j \in 0\ ..\ N$

  for $k \in 0\ ..\ NZ$

    $Ac_{j\ ,k} \leftarrow act$

for $t \in 0\ ..\ NT$

  "obtain steady state profiles at time t"

  $(\omega\ \ \theta f\ \ p\ ) \leftarrow Rxt2D(Ac\ ,NZ)$

  "bulk composition at exit for time t"

  for $n \in 0\ ..\ NC-1$

    $\omega\_exit_{n\ ,t} \leftarrow \omega_{n\ ,NZ}$

  "compute particle temperatures"

  $\theta f_{col} \leftarrow submatrix(\theta f\ ,0\ ,N-1\ ,0\ ,NZ)$

  for $k \in 0\ ..\ NZ$

    for $j \in 0\ ..\ N-1$

      $rdisp_{j\ ,k} \leftarrow \alpha_{Hp} \cdot \left[\sum_{i=0}^{N-1} \left(B_{j\ ,i} \cdot \theta f_{col_{i,k}}\right) + B_{j\ ,N} \cdot \theta_N\left(\theta f_{col}{}^{\langle k \rangle}\right)\right]$

      $tp \leftarrow \theta_0$

      $\theta p_{j\ ,k} \leftarrow root\left(ftp\left(tp\ ,\theta f_{j\ ,k}\ ,p_k\ ,\omega^{\langle k \rangle}\ ,Ac_{j\ ,k}\ ,rdisp_{j\ ,k}\right),tp\right)$

    ""

$\theta p_{N,k} \leftarrow \theta_N\left(\theta p^{\langle k \rangle}\right)$

" update the activity"

for $j \in 0 .. N$

for $k \in 0 .. NZ$

$Ac_{j,k} \leftarrow Ac_{j,k} + h \cdot decay\left(Ac_{j,k}, \theta p_{j,k} \cdot T_0, T_s, k_d\right)$

"activity must not be negative"

$Ac_{j,k} \leftarrow max\left(Ac_{j,k}, 0\right)$

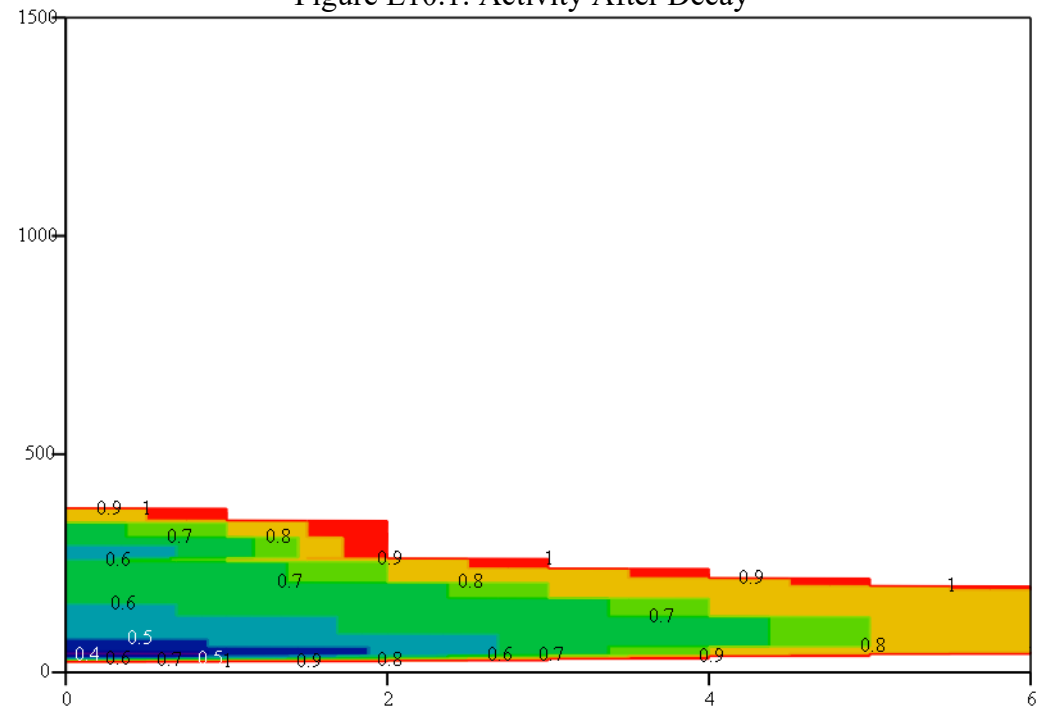
$(Ac \quad \omega\_exit \quad \theta p)$

$tf := \dfrac{10}{k_d} = 7.2 \times 10^4 s \quad tf = 20 \cdot hr$ final time $NT := 50$ number of time steps

$act := 1$

$(Ac \quad \omega\_exit \quad \theta p\_after) := Age\left(act, NT, tf, T_s, k_d, NZ\right)$

Figure E10.1: Activity After Decay



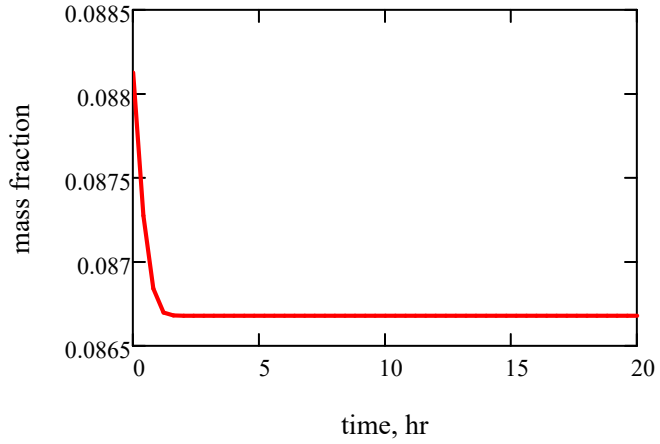
Ac

lowest activity in the reactor

$min(Ac) = 0.328$

$t := 0 .. NT$ $\quad$ $t\_age_t := \frac{t \cdot tf}{NT}$

Fig E10.2: Formaldehyde in Effluent



Observation:
The damage to the catalyst due to sintering has not severely affected the conversion.

exit composition before decay

$$\omega z(1) = \begin{pmatrix} 5.887 \times 10^{-3} \\ 0.063 \\ 0.062 \\ 6.25 \times 10^{-3} \\ 0.088 \\ 0.775 \end{pmatrix}$$

exit composition after decay

$$\omega\_exit^{\langle NT \rangle} = \begin{pmatrix} 7.568 \times 10^{-3} \\ 0.064 \\ 0.061 \\ 6.13 \times 10^{-3} \\ 0.087 \\ 0.775 \end{pmatrix}$$

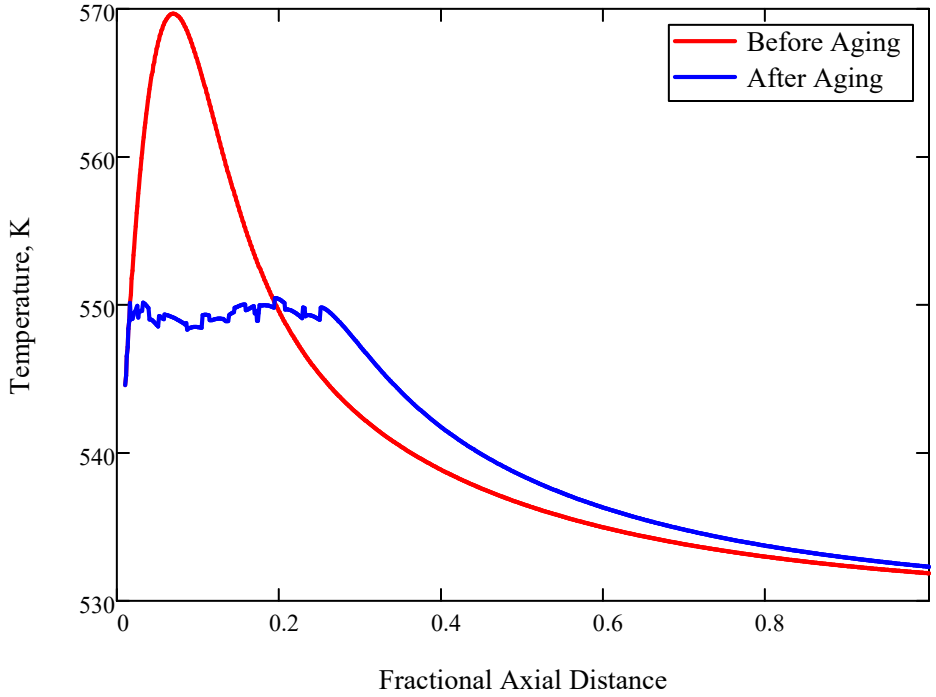
$$dp\_after_k := \left(Q^{-1} \cdot \theta p\_after^{\langle k \rangle}\right)$$

polynomial coefficients for particle temperatures

$$Tp_{col\_after}(k, r) := T_0 \cdot \sum_{i=0}^{N} \left[\left(dp\_after_k\right)_i \cdot r^{2 \cdot i}\right]$$

$Tp\_after(z,r) := Tp_{col\_after}(round(z \cdot NZ), r)$ particle temperatures in terms of axial and radial fractions

Fig. E10.3: Centerline Temperatures Before and After Aging



Decay options

Other decay mechanisms with large time constants can be explored in a similar manner. For example, the *Age* program could be written to track the accumulation of a poison with an adsorption term at each location. The steady state program would still be used to update the composition and temperature profiles without the need for a full dynamic model involving the adsorption process.

References: see Example 7