

# Non dimensionalization of frontal polymerization equations and mesh adaptivity notes

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## Abstract

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*Keywords:*

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## 1. Nomenclature

Symbols

$\alpha$	State variable representing degree of cure (dimensionless)
$A$	Pre-exponential factor ( $s^{-1}$ )
$C_p$	Specific heat (J/kg-K)
$E$	Activation energy (J/mol)
$H_r$	Heat of reaction (J/kg)
$K_{cat}$	Coefficient used in autocatalytic model (dimensionless)
$k$	Thermal conductivity (W/m-K)
$R$	Universal gas constant, 8.314 J/mol-K
$\rho$	Density ( $kg/m^3$ )
$T_o$	Initial temperature (K)
$T_{trig}$	Ignition temperature (K)
$\tau$	Non-dimensional time

## 2. Equations in dimensional form

The equations are

$$f(\alpha) = (1 - \alpha)^n(1 + K_{cat}\alpha) \quad (1)$$

$$\frac{d\alpha}{dt} = A \cdot \exp\left(\frac{-E}{RT}\right) \cdot f(\alpha) \quad (2)$$

$$k\nabla^2 T + \rho H_r \frac{d\alpha}{dt} = \rho C_p \frac{\partial T}{\partial t} \quad (3)$$

### 3. Non dimensional equations

Let non-dimensional time  $\tau = A \cdot t$ , and non-dimensional temperature be

$$\theta = \frac{T - T_o}{T_{trig} - T_o} \quad (4)$$

where  $T_o$  is initial temperature,  $T_{trig}$  is ignition temperature.

Using Eq. 3, and ignoring the diffusion term, a simple calculation shows that:

$$\rho H_r \frac{1 - 0}{\Delta t} = \rho C_p \frac{T_{trig} - T_o}{\Delta t} \quad (5)$$

Which leads to the choice of  $T_{trig}$  as:

$$T_{trig} = T_o + H_r / C_p \quad (6)$$

Using the microchannel radius  $R_m$  as the scaling factor for both z and r co-ordinates, the equations can be non-dimensionalized as:

Heat conduction equation:

$$\left[ \frac{k}{\rho C_p A R_m^2} \right] \nabla^2 \theta + \left[ \frac{H_r}{C_p (T_{trig} - T_o)} \right] \frac{d\alpha}{d\tau} = \frac{\partial \theta}{\partial \tau} \quad (7)$$

Which by virtue of Eq. 7 becomes:

$$\left[ \frac{k}{\rho C_p A R_m^2} \right] \nabla^2 \theta + [1] \frac{d\alpha}{d\tau} = \frac{\partial \theta}{\partial \tau} \quad (8)$$

The cure equation is:

$$\frac{d\alpha}{d\tau} = \exp \left( \frac{-E}{R(\theta(T_{trig} - T_o) + T_o)} \right) \cdot f(\alpha) \quad (9)$$

As per [1] the values for medium catalyst concentration are:

$$A = 1.91e5 \text{ s}^{-1} \quad (10)$$

$$E = 51.1 \text{ kJ/mol} \quad (11)$$

$$n = 1.927, \quad K_{cat} = 0.365 \quad (12)$$

The DCPD material properties are:

$$k = 0.152 \text{ W/m-K} \quad (13)$$

$$\rho = 980 \text{ kg/m}^3, \quad C_p = 1440 \text{ J/kg/K}, \quad H_r = 460 \text{ kJ/kg} \quad (14)$$

## 4. Notes on mesh adaptivity

### 4.1. Gradient jump indicator

The file `GradientJumpIndicator.C` in the MOOSE documentation gives an idea of the indicator. Elements with linear shape function have a constant gradient, the gradient jump is basically the difference in the gradient between a given element and its neighbours. The indicator file returns the square of this gradient jump.

### 4.2. Working of the error fraction marker

At each time step, the error for each element is calculated. The error is the indicator chosen by the user (it could be gradient jump, or the other indicators defined in MOOSE).

The user inputs the ‘coarsen’ and ‘refine’ parameters. Both these can have values between 0 and 1 independent of each other.

The maxima and minima of these values is calculated. Let’s call it ‘max’ and ‘min’.

$$\Delta = max - min \quad (15)$$

$$refine\_cutoff = (1 - refine) * max \quad (16)$$

$$coarsen\_cutoff = coarsen * \Delta + min \quad (17)$$

If the error is more than the refine cut-off, then the element is refined. If less than the coarsen cut-off then the element is coarsened, nothing is done if none of these two conditions are met.

The above logic is implemented in `ErrorFractionMarker.C` file.

## References

- [1] Kessler, M.R., White, S.R.. Cure kinetics of the ring-opening metathesis polymerization of dicyclopentadiene. *Journal of Polymer Science Part A: Polymer Chemistry* 2002;40(14):2373–2383.