SIMULATION OF ROTATIONAL MOLDING

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INTRODUCTION

Non-reactive rotational molding

Reactive rotational molding
There are not any chemical reactions during rotomolding.

The transformation is based essentially on physical state changes.

The polymer is as powder (100-500µm)

Examples: thermoplastics (PE, PP, PA, PC,...)
There are chemical reactions during this processing.

- Examples: Thermosets, rubbers, polymerization of certain polymers (PA6) chemical modification of certain polymers.
DIFFERENT STEPS OF SIMULATION

**Reactive rotational molding**
- Chemical reactions (cross-linking, polymerization)
- Rheology
- Flow of liquid mixture

**Non-reactive rotational molding**
- Flow of particles (powder)?
- Sintering
- Melting
- Rheology
- Flow of melted (viscous) polymer
- Solidification (crystallization)

Heat transfer
CYCLE TIME

T (°C)

solid

Molten polymer

solid+molten polymer

solid+molten polymer

solid

I II III IV V

time (min)

↑ solid

↑ 10

↑ 20

↑ 30

↑ 40
HEAT TRANSFER
1. *Convection* air of oven / metallic surface of the mold
2. *Conduction* in the thickness of the mold
3. Transmission mold / polymer
4. *Conduction* in the thickness of the molten polymer layer
5. *Convection* polymer / mixture of air and powder
HEAT TRANSFER

1 - Convection air of oven / metallic surface of the mold

\[ -k_m \left( \frac{\partial T}{\partial x} \right) = h_{ov/m} (T_{ov} - T) \]

2 - Conduction in the thickness of the mold

\[ \rho_m \ C_{pm} \left( \frac{\partial T}{\partial t} \right) = \frac{\partial}{\partial x} \left( k_m \frac{\partial T}{\partial x} \right) \]

3 - Transmission mold / polymer

\[ -k_m \left( \frac{\partial T}{\partial x} \right) = -k_p \left( \frac{\partial T}{\partial x} \right) \]

4 - Conduction in the thickness of the molten polymer layer

\[ \rho_p \ C_{pp} \left( \frac{\partial T}{\partial t} \right) + \Delta H = \frac{\partial}{\partial x} \left( k_p \frac{\partial T}{\partial x} \right) \]

5 - Convection polymer / mixture of air and powder

\[ -k_p \left( \frac{\partial T}{\partial x} \right) = h_{pa} (T_{pa} - T) \]
RESULTS

Evolution de $T_a$ pour les trois conditions opératoires choisies. Comparaison des courbes expérimentales et numériques ($T_{four} = 300 \, ^\circ C$, $t_{chauffe} = 20, 25$ et $30$ min).
Rheochemistry and rheokinetic of thermosets during rotational molding

**Chemistry**
- Cross-linking mechanism
- Kinetic models

**Rheology**
- Evolution of viscosity
- Rheological models

**Fluid Mechanic**
- Fluid flow models
- Finite elements and SPH

Heat transfer

Experimental methods, DSC, IR spectrophotometry, Rheometry
Cross-linking reaction

\[- \frac{d[E]}{dt} = [E]_0[A]_0(1 - x)^2 \times (k' + k(\text{[OH]}_0 + x[E]_0) + k''[HX])\]

Rheology

\[\eta = \left(\frac{x^*}{x^* - x}\right)^{A + B\alpha}\]

\[\frac{\eta}{\eta_0} = \left(\frac{x^*}{x^* - x}\right)^{A + B\alpha}\]
SPH is a Lagragian method for simulation of fluid flow. In this method the material at macroscopic scale is considered as a group of particles of mass $m_i$, rate $v_i$ avec other properties like pressure, $p_i$, temperature, $T_i$, internal energy $U_i$, entropy $S_i$, …

- Central function
- Smoothing length
- Conservation of quantity of movement
- Conservation of energy
- Equation of state
- Density
- Schema of integration
A cylindrical mold turning around its principal axis
SIMULATION OF FLUID FLOW

A part with more complex geometry
Cubic mold in rotomolding condition
NON-REACTIVE
ROTATIONAL MOLDING
FORMATION OF DIFFERENT LAYERS

Melting + Coalescence

Layer by Layer

Particle (polymer)

1st layer

Molten Polymer

2nd layer

3th layer

4th layer
The following schema shows the mechanism of melting of a particle and its adhesion on the internal surface of the mold.

The particles fall on the bottom of the mold, will be melted progressively and spread on the internal surface. This spreading depends on the force of gravity and the surface tension.
The shear force induced by the weight of particle assures the adhesion between melted particle and the surface of the mold. On the superior part of the mold, the surface tension spreads the melted polymer on the surface.
NON-REACTIVE ROTATIONAL MOLDING

- Flow of particles (powder)?
- Sintering (coalescence + densification)

Different steps of coalescence de grains
1) initial state
2 and 3) growth
4) final state
DIFFERENT MODELS

- Frenkel

\[ \frac{x^2}{r} = \frac{3}{2} \left( \frac{\gamma}{\eta} \right) t \]

- Kuckzynski

\[ \left( \frac{x^2}{r^{1.02}} \right)^n = K(T)t \]

- Eshely

\[ \frac{X}{a} = \left( \frac{\gamma t}{\eta a_0} \right)^{1/2} \]

- Lontz

\[ \frac{x^2}{r} = \frac{3}{2} \left( \frac{\lambda}{\eta_0 \left( 1 - e^{\frac{-r}{\tau}} \right)} \right) t \]
**Example: PVDF**

- Under optical microscope

![Images of PVDF samples at different times and temperatures.](image-url)
Example: PVDF
NON-REACTIVE ROTATIONAL MOLDING

- Melting
- Rheology
- Flow of molten (viscous) polymer
- Solidification (crystallization)
Reactive rotational molding

- Chemical reactions
  - Kinetic model
- Heat transfer
  - $T = f(t)$
- Rheology
  - $\eta = f(t)$
- $\eta = f(x)$
- Fluid flow model

X: degree of conversion
CONCLUSION
Non-reactive rotational molding

Non-reactive rotational molding

Heat transfer
$T = f(t)$

Melting

X: degree of conversion

Formation of layers

Densification

Rheology

fluid flow model

Cooling

Solidification crystallization

Coalescence
Kinetic model