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Numerical study of the plastification of an amorphous polymer in a hot end extruder of a 3D printer

F. Pigeonneau, M. Vincent & J.-F. Agassant (Mines-ParisTech PSL - CE-MEF)



1. Introduction

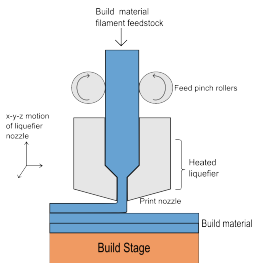


FIGURE 1 – Sketch of the fused deposition modelling process.

1. Introduction

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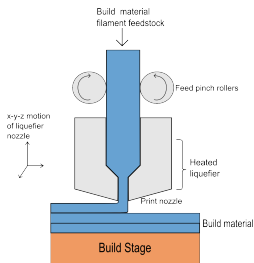


FIGURE 1 – Sketch of the fused deposition modelling process.

non isothermal process

1. Introduction

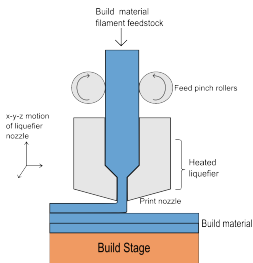


FIGURE 1 – Sketch of the fused deposition modelling process.

non isothermal process

- ▶ What is the temperature history through the hot end extruder ?
- ▶ How does the inlet velocity impact temperature history ?
- ▶ What is the residence time distribution in the hot end extruder ?

1. Introduction

2. Problem statement

3. Thermal behavior

3.1 Comparison to Peng et al. experiment

3.2 Effect of the inlet velocity

4. Kinematic behavior

4.1 Velocity profiles

4.2 Residence time

5. Conclusion and future works

2. Problem statement

- Geometry taken according to Peng et al. ¹.

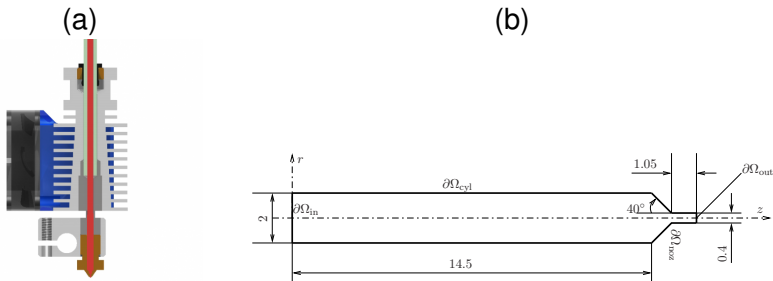


FIGURE 2 – (a) E3D-v6 hot-end liquefier (<https://e3d-online.com/>) and (b) geometry used in the numerical computations (dimensions in mm).

1. F. PENG/B. D. VOGT/M. ÇAKMAK : Complex flow and temperature history during melt extrusion in material extrusion additive manufacturing, in : *Addit. Manuf.* 22 (2018), p. 197-206, URL : <https://www.sciencedirect.com/science/article/pii/S2214860417303718>.

2. Problem statement

- ▶ As in Peng et al., the polymer is the bisphenol-A polycarbonate (Makrolon[®] 3208)².

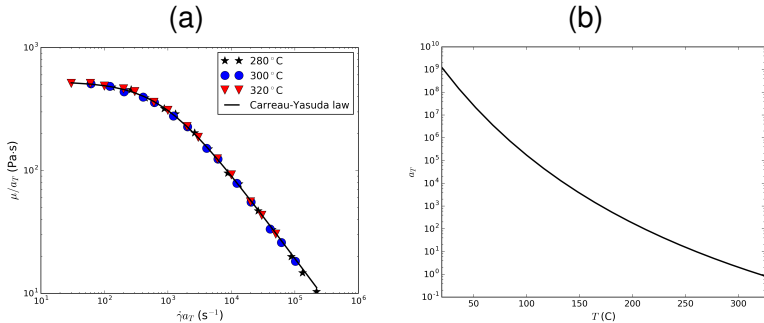


FIGURE 3 – (a) μ/a_T vs. $a_T\dot{\gamma}$ and (b) a_T vs T .

2. Problem statement

- ▶ Mass balance equation :

$$\nabla \cdot \mathbf{u} = 0. \quad (1)$$

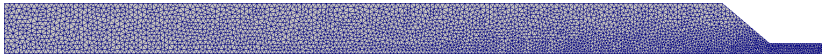
- ▶ Momentum balance equation :

$$\nabla \cdot [2\mu(\dot{\gamma}, T)\mathbf{D}] - \nabla P = 0. \quad (2)$$

- ▶ Energy balance equation :

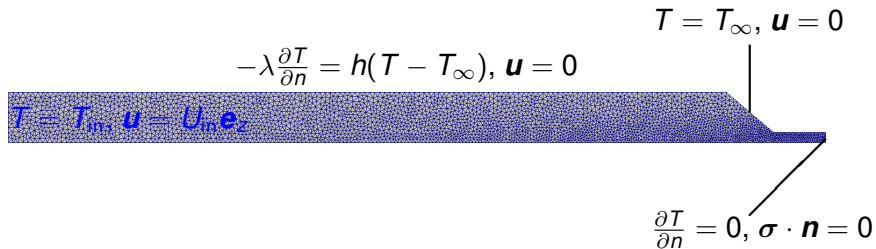
$$\rho C_p \frac{DT}{Dt} = \lambda \nabla^2 \theta + \mu(\dot{\gamma}, \theta) \dot{\gamma}^2. \quad (3)$$

2. Problem statement



2. Problem statement

7



2. Problem statement

- ▶ h depends on the air thermal resistance between the filament and the hot end extruder :

$$h \sim \frac{\lambda_{\text{air}}}{e_{\text{air}}} = 200 \text{ W}/(\text{m}^2\text{K}). \quad (4)$$

- ▶ To be in agreement with experiments of Peng et al.³ :
 - ▶ $T_{\text{in}} = 24^\circ\text{C}$;
 - ▶ $T_{\infty} = 325^\circ\text{C}$.

3. PENG/VOGT/CAKMAK : Complex flow and temperature history during melt extrusion in material extrusion additive manufacturing (cf. note 1).

3. Thermal behavior

3.1 Comparison to Peng et al. experiment

- Peng et al.⁴ measured the thermal history by introducing a thermocouple in the filament.

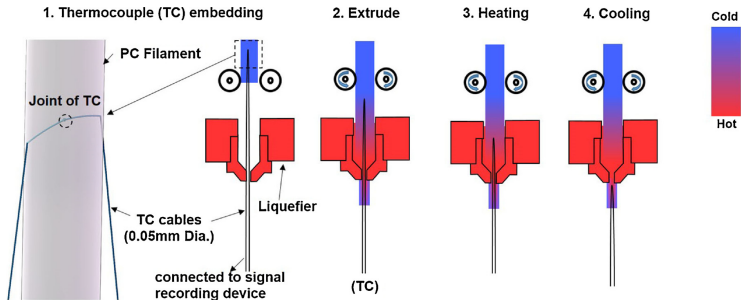


FIGURE 4 – Experimental set-up of Peng et al.

4. PENG/VOGT/CAKMAK : Complex flow and temperature history during melt extrusion in material extrusion additive manufacturing (cf. note 1).

3. Thermal behavior

3.1 Comparison to Peng et al. experiment

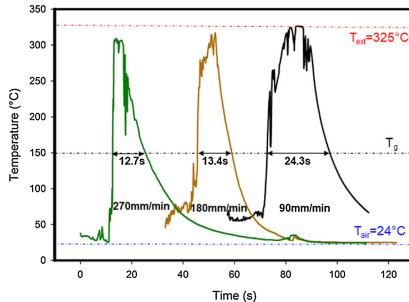


FIGURE 5 – T vs. t recorded by thermocouples [Peng et al. (2018)].

3. Thermal behavior

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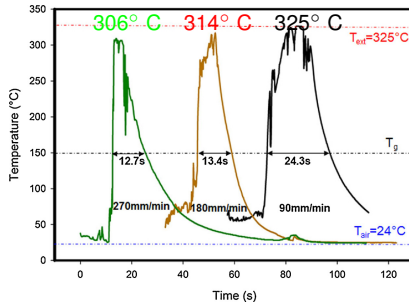


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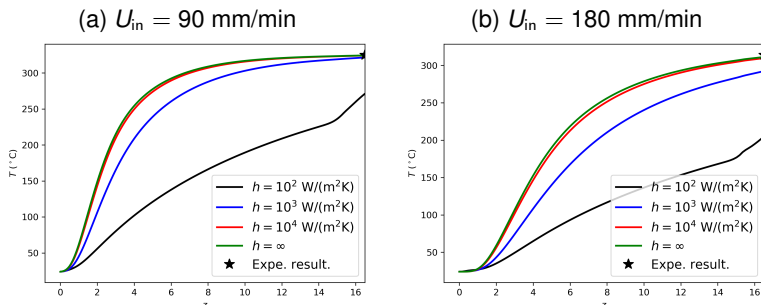


FIGURE 6 – T vs. z in $r = 0$ for (a) $U_{in} = 90$ mm/min and (b) $U_{in} = 180$ mm/min.

3. Thermal behavior

3.1 Comparison to Peng et al. experiment

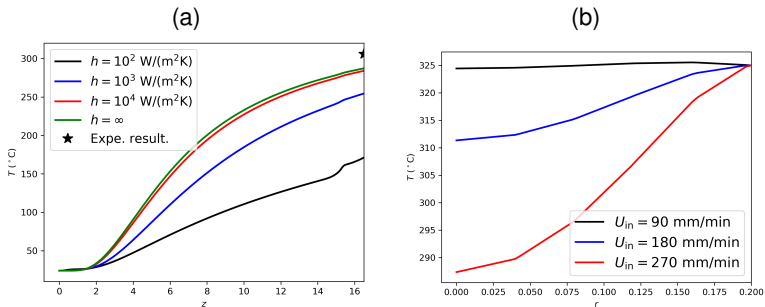


FIGURE 7 – (a) T vs. z in $r = 0$ for $U_{in} = 270$ mm/min (b) T vs. r at the exit.

3. Thermal behavior

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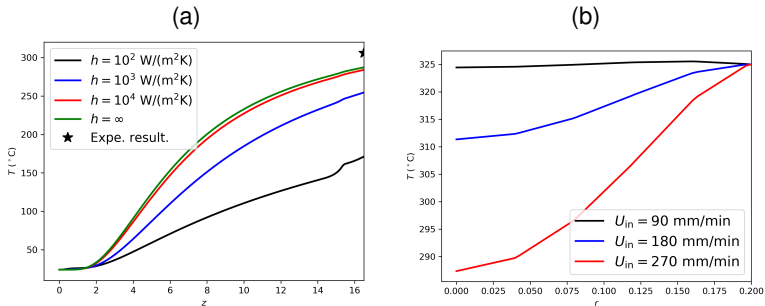


FIGURE 7 – (a) T vs. z in $r = 0$ for $U_{in} = 270$ mm/min (b) T vs. r at the exit.

→ **Heat transfer between the hot end extruder and the polymer very efficient**

3. Thermal behavior

3.2 Effect of the inlet velocity

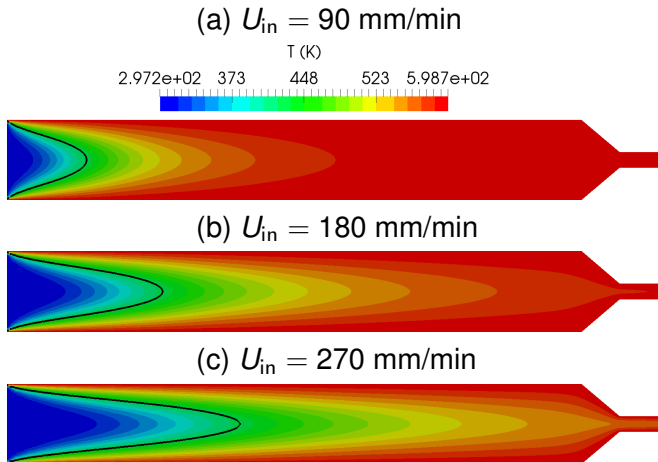


FIGURE 8 – T field in Kelvin for three U_{in} .

3. Thermal behavior

3.2 Effect of the inlet velocity

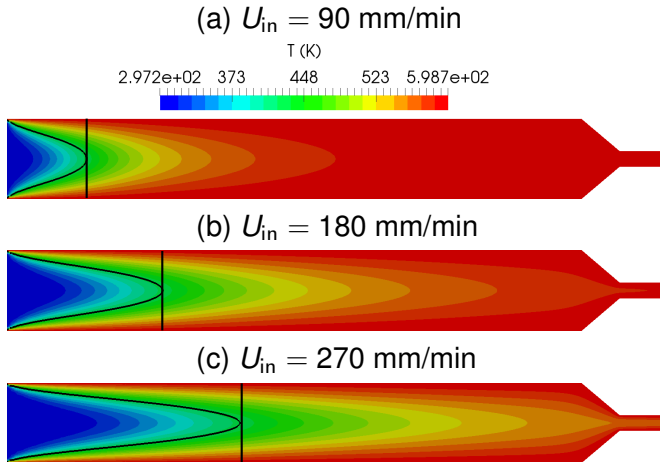


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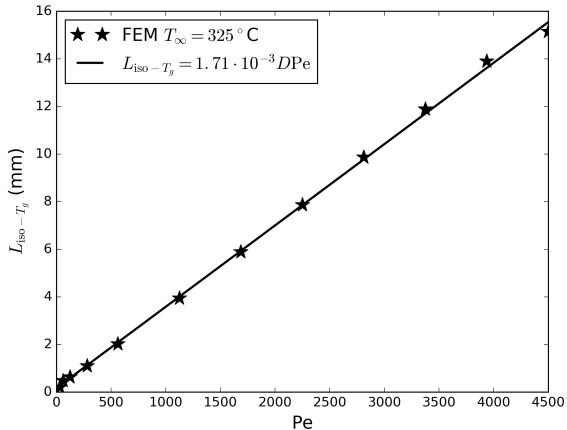


FIGURE 9 – $L_{\text{iso}-T_g}$ vs. $Pe = UD/\kappa$.

3. Thermal behavior

3.2 Effect of the inlet velocity

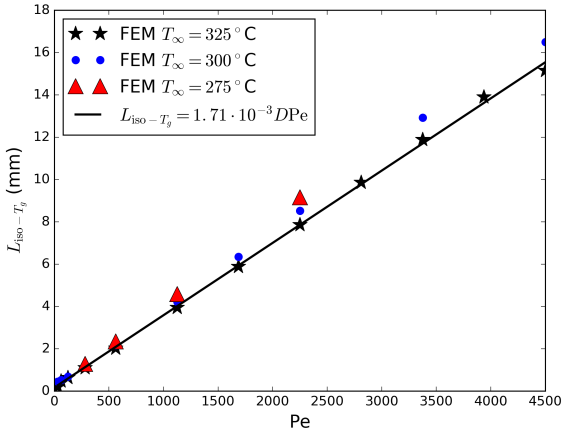


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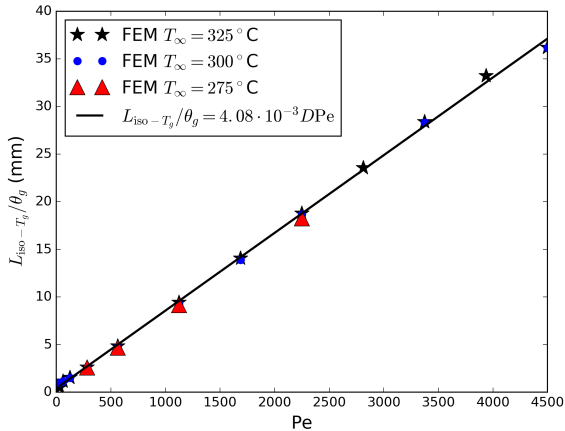


FIGURE 9 – $L_{\text{iso}-T_g}(T_{\infty} - T_{\text{in}})/(T_g - T_{\text{in}})$ vs. $Pe = UD/\kappa$.

3. Thermal behavior

3.2 Effect of the inlet velocity

- ▶ This result shows that

$$\frac{T_{\infty} - T_{in}}{T_g - T_{in}} = 4.08 \cdot 10^{-3} \frac{UD^2}{\kappa L}. \quad (5)$$

$$U_{in} = \frac{9.804 \lambda L}{\rho C_p D^2} \frac{T_{\infty} - T_{in}}{T_g - T_{in}}. \quad (6)$$

- ▶ The inlet velocity decreases with T_g .
- ▶ The inlet velocity increases with T_{∞} :
 - ▶ $T_{\infty} = 275^{\circ}\text{C}$, $U_{in} = 644$ mm/min ;
 - ▶ $T_{\infty} = 300^{\circ}\text{C}$, $U_{in} = 708$ mm/min ;
 - ▶ $T_{\infty} = 325^{\circ}\text{C}$, $U_{in} = 773$ mm/min.

4. Kinematic behavior

4.1 Velocity profiles

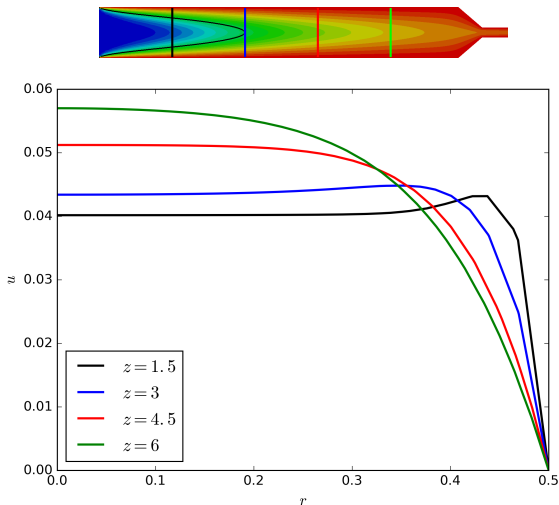


FIGURE 10 – u vs. r in dimensionless units for $U_{in} = 270$ mm/min.

4. Kinematic behavior

4.2 Residence time

- ▶ The residence time distribution is determined by⁵

$$E(t) = \frac{dF(t)}{dt}, \quad (7)$$

with

$$F(t) = \frac{\int_{\partial\Omega_{\text{out}}} C \mathbf{u} \cdot \mathbf{n} dS}{\int_{\partial\Omega_{\text{out}}} \mathbf{u} \cdot \mathbf{n} dS}. \quad (8)$$

- ▶ C is solution of

$$\frac{\partial C}{\partial t} + \nabla C \cdot \mathbf{u} = 0, \quad (9)$$

with

$$C(\mathbf{x}, 0) = 0, \quad \forall \mathbf{x} \in \Omega, \quad (10)$$

$$C(\mathbf{x}, t) = 1, \quad \forall \mathbf{x} \in \partial\Omega_{\text{in}}. \quad (11)$$

5. P. V. DANCKWERTS : Continuous flow systems. Distribution of residence times, in : Chem. Eng. Sci. 2 (1953), p. 1-13.

4. Kinematic behavior

4.2 Residence time

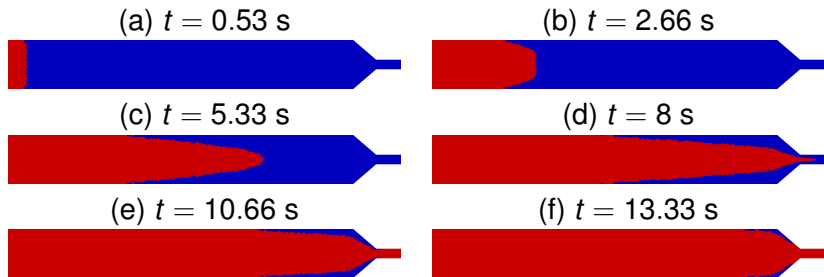


FIGURE 11 – Snapshots of C for $U_{in} = 90$ mm/min.

4. Kinematic behavior

4.2 Residence time

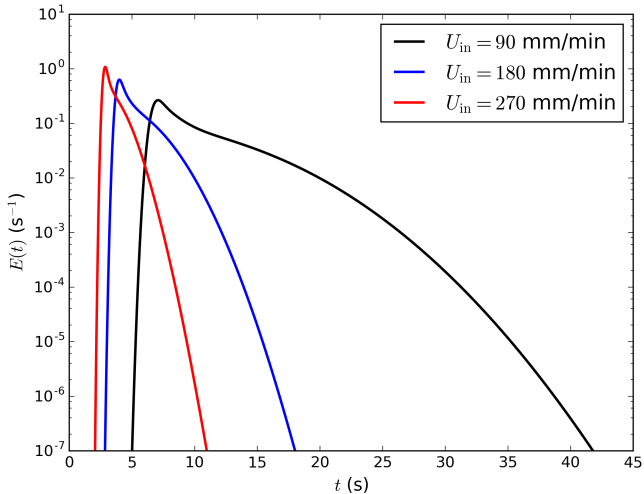


FIGURE 12 – E (s^{-1}) vs. t (s).

4. Kinematic behavior

4.2 Residence time

- ▶ According to Villiermaux⁶, normalization by $t_{\text{geo}} = V/Q$.

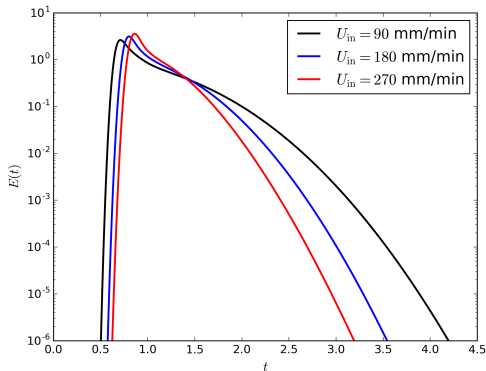


FIGURE 13 – E vs. t .

4. Kinematic behavior

4.2 Residence time

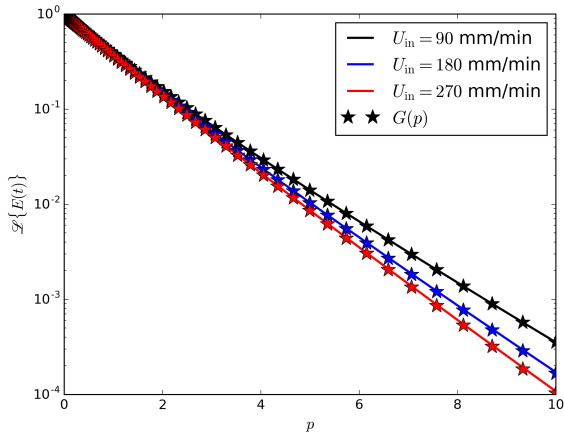


FIGURE 14 – $\mathcal{L}\{E(t)\}$ vs. p .

4. Kinematic behavior

4.2 Residence time

$$G(p) = \frac{\exp(-\tau_1 p)}{1 + \tau_2 p},$$

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FIGURE 15 – Plug flow reactor (PFR).

$$E(t) = \delta(t - \tau_1). \quad (12)$$

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FIGURE 15 – Plug flow reactor (PFR).

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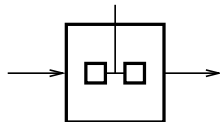


FIGURE 16 – Continuous stirred tank reactor (PFR).

$$E(t) = \frac{1}{\tau_2} \exp\left(-\frac{t}{\tau_2}\right). \quad (13)$$

4. Kinematic behavior

4.2 Residence time

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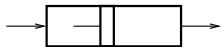


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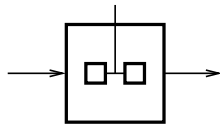


FIGURE 16 – Continuous stirred tank reactor (PFR).

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$G(p)$ similar to the function of Bellini et al.⁷.

7. A. BELLINI/S. GUCERI/M. BERTOLDI : Liquefier dynamics in fused deposition, in : J. Manuf. Sci. Eng. 126.2 (2004), p. 237-246.

4. Kinematic behavior

4.2 Residence time

U_{in}	τ_1	τ_2
90 mm/min	0.632 6.30 s	0.405 4.03 s
180 mm/min	0.729 3.63 s	0.307 1.53 s
270 mm/min	0.795 2.64 s	0.241 0.80 s

TABLE 1 – τ_1 and τ_2 of a PFR mixer in serial with CSTR mixer.

5. Conclusion and future works

- ▶ Heat & mass transfer are solved numerically with the thermal and shear rate dependence in μ .
- ▶ Using the same working conditions of Peng et al.⁸, we argue :
 - ▶ the heat transfer coefficient is important → very efficient contact between the hot end extruder and the polymer ;
 - ▶ the presence of a plug flow mainly upstream where $T < T_g$.
- ▶ The determination of the iso- T_g spreading allows to define the limit of the liquefier in terms of flow rate.
- ▶ The residence time distributions show :
 - ▶ the hot-end extruder is equivalent to a plug flow reactor and a continuous stirred tank reactor in serial.
 - ▶ The importance of the plug flow reactor increases with the inlet velocity.

8. PENG/VOGT/CAKMAK : Complex flow and temperature history during melt extrusion in material extrusion additive manufacturing (cf. note 1).

5. Conclusion and future works

- ▶ Reproduce the same study for another polymer (for instance ABS).
- ▶ Introduce a more realistic constitutive law to describe the solid to fluid transition.
- ▶ Study the hot-end extruder on the whole.
- ▶ Describe the thermal transfer during the deposition.

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