Simulations And Injection Molding Experiments For Aluminum Nitride Feedstock

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Abstract

Powder injection molding (PIM) simulations are useful for predicting mold-filling behavior because they aid in material, process and part design. To perform PIM simulations, measurements for feedstock properties such as physical, thermal, and rheological are required as input parameters. The availability of data for such feedstock properties is limited and fresh measurements are often required in order to perform PIM simulations for variations in feedstock composition. A recent study by our group presented a procedure to estimate feedstock properties and use them in mold-filling simulations. The present work compares the predictions of PIM mold-filling simulations using experimental and estimated feedstock properties with injection-molding experiments. Aluminum nitride (AlN) feedstock of 80.5 wt.% was compounded using a twin-screw extruder and injection-molded as tensile bars. Injection-molding experiments were performed using the AlN feedstock at various melt temperatures and injection pressures to obtain complete and partially filled parts. Simulations were performed using measured and estimated AlN feedstock properties on the tensile-bar geometry used during injection molding experiments. Melt temperature was varied while performing simulations to obtain a process window for complete and partially filled parts.

A comparison between injection molding experiments and simulations was made to understand the dependence of the estimated and experimental feedstock properties in predicting mold filling behavior.

1. Introduction

Powder injection molding (PIM) is a multi-step process that can be divided into four basic steps: 1) ceramic or metal powders are mixed with polymer binders to form a homogenous feedstock using a twin-screw extruder, 2) the feedstock is injection molded into desired geometries using an injection molding machine, 3) the binder phase is debound from the molded parts by thermal or solvent based techniques, and 4) debound parts are sintered to achieve final parts. The PIM simulations are generally performed typically after feedstock compounding to identify appropriate process and geometry attributes for optimum molding [1]–[12]. Common injection molding simulation tools include Autodesk Moldflow, Sigmasoft, PIMsolver, and Modlex3D.

To perform PIM simulations, feedstock property measurements for density, thermal conductivity, and specific heat are required for a range of temperatures. Further, viscosity measurements are required for a range of shear rates and temperatures, and specific volume measurements are required for a range of temperatures and pressures [1–4]. Availability of such feedstock property data is limited and properties are typically measured for a particular composition.

A recent work by our group suggests a design method that uses empirical equations and estimate feedstock properties as a function of composition, filler properties, and binder properties [17]. This design method employs the use of available literature filler and binder properties to estimate physical, thermal and rheological properties for nine different ceramic feedstocks [17]. An extension of this work outlines a procedure to use feedstock property estimates in mold-filling simulations [18].

In the current work, 80.5-weight percent aluminum nitride (AlN) feedstock was extruded and injection molded into a tensile bar geometry. Injection molding was performed as a function of melt temperature and injection pressure in order to obtain parts with partial

and complete mold filling. Feedstock properties for AlN were measured at Datapoint Labs and estimated using our design procedure for PIM simulations [5, 6]. To perform PIM simulations a tensile bar geometry was designed according to the mold tool dimensions. Simulations were performed using measured and estimated AlN feedstock properties at various melt temperatures and injection pressures to obtain complete and partially filled parts. Comparisons of melt temperatures from simulation and experiments were made to understand the effectiveness of PIM simulations in predicting mold-filling behavior.

2. Experimental Methods

Commercially available aluminum nitride (AlN) powder (median particle size of 1 μm) and a wax-polymer binder were used as starting materials. The binder is composed of paraffin wax, low-density polyethylene, polypropylene, and stearic acid. Details of the binder composition and feedstock compounding are provided [19], [20]. A feedstock with 80.5 wt.% AlN powder was compounded using a 27 mm twin-screw extruder with a length to diameter (L/D) ratio of 40.

Material property measurements were made at Datapoint Labs (Ithaca, NY) for the AlN feedstock and a wax-polymer binder [7, 8]. Solid density measurements were made for AlN feedstock and wax-polymer binder using Archimedes principle as laid out in ASTM standard D792. The melt density measurement was done using a Gottfert Rheograph capillary rheometer in accordance with ASTM D3835 for AlN feedstock and a wax-polymer binder. A Perkin Elmer differential scanning calorimetry (DSC) was used to measure specific heats for AlN feedstock and a wax-polymer binder in accordance with ASTM E1269 standard. Thermal conductivity measurements for AlN feedstock and the wax-polymer binder were made using a K-System II thermal conductivity system in accordance with ASTM standard D5930. Viscosity for AlN feedstock and the wax-polymer binder was measured according to ASTM D3835 using a Gottfert Rheograph capillary rheometer. Pressure-volume-temperature (PVT) measurements for AlN feedstock and the wax-polymer binder were made with a Gnomix PVT apparatus in accordance with ASTM D792 [7, 8]. The feedstock property measurements were

compared to values estimated using models listed in **Table 1**. Description of the symbols used in **Table 1** and throughout this paper is presented in **Table 2**.

The AIN feedstock was injection molded into a tensile bar geometry using an Arburg 221M injection-molding machine. An injection gate with a size of 6.5 mm was used to inject the AIN feedstock into the mold cavity. Injection molding experiments were performed at a set of melt temperatures and injection pressures to obtain parts with complete and incomplete mold fill (**Table 3**). In the first molding experiment (**Table 3**) the injection pressure (P_i) was set at 38 MPa and melt temperature (T_m) was set at 455 K. A total of 50 parts with no defects were molded during this experiment and a specimen part is shown in **Figure 1a**. To understand the effect of decreases in injection pressure and melt temperature on the molding behavior, experiments # 2-4 were performed (**Table 3**). For Experiments 2-4 the melt temperatures was decreased from 444 K to 422 K while keeping injection pressure constant at 14 MPa to obtain parts with incomplete mold fill (short shot). A total of four to five specimens were injection molded in each of the experiments 2-4 and sample molded specimens are presented in **Figure 1b-d**. All injection molding experiments listed in **Table 3** were performed at injection speed of 33 cm³/s, the initial packing pressure was set at 100% of the injection pressure value for the first second and then it was reduced to 65% of the injection pressure value for the next 1.2 s. To calculate the percentage of part filled of the incompletely filled samples, their weights were compared to those of the filled samples.

To perform mold-filling simulations, the tensile bar geometry model was imported into the Autodesk Moldflow software. The tensile bar geometry was meshed using an automated solid 3D meshing protocol based on finite element analysis. A gate size of 6.5 mm was set to perform molding simulations. A fill-and-pack type process module was selected to perform simulations. Simulations were performed using measured and estimated AIN feedstock property values.

Simulations were performed on a 3D tensile bar geometry model designed using Solidworks in accordance with the mold tool dimensions. The dimensions for the tensile bar geometry are shown in **Figure 2**. Initial simulations were performed using Autodesk Moldflow software for injection molding conditions listed in **Table 3**. Additional

simulations for lower values of melt temperature were performed in case short shots were not obtained at the melt temperature of 422 K.

3. Results and Discussion

3.1. Properties

The physical, thermal and rheological properties of AIN feedstock were estimated using selected empirical models presented in **Table 1**. The empirical models estimate material properties of feedstocks as a function of feedstock composition and filler and binder properties. The empirical models were selected by performing an in-depth statistical analysis on various published models that were fitted to literature data on experimentally-measured properties of powder-polymer mixtures [13]. The thermal, physical and rheological properties of the wax-polymer binder and thermal and physical properties of AIN filler were collected from literature. Filler properties collected from literature were reported for 300 K.

The solid and melt density of AIN feedstock was estimated using **Equation 1** for 22 data points of AIN filler density ($3300 \pm 50 \text{ kg/m}^3$) [13–27]. Estimations were made for the wax-polymer solid and melt density values of 870 and 700 kg/m^3 respectively and details for estimation procedure are reported elsewhere [17–19, 33]. The experimentally measured and estimated values of solid and melt densities for the AIN feedstock are presented in **Table 4**. The average values of density estimates and measured values of density from **Table 4** were used to create a dataset necessary for performing mold-filling simulations.

Furthermore, the densities values of AIN filler and the wax-polymer binder in conjunction with **Equation 2** and **3** were used to calculate volume fraction of the AIN feedstock. Volume fraction values are required to estimate feedstock properties such as viscosity and thermal conductivity.

The specific heat of the AIN feedstock was estimated using **Equation 4** as a function of temperature for six data points of filler specific heats ($800 \pm 30 \text{ J/kg.K}$) [34–36]. Estimations were made for the wax-polymer binder specific heats reported for temperatures between 283 and 430 K. The specific heat values of the wax-polymer

binder used for this estimation ranged between 2080 and 4640 J/kg.K and details for the estimation procedure are reported elsewhere [17–19, 33]. The experimentally measured and estimated values of specific heats for the AIN feedstock are presented in **Table 5**. The average values of specific heat estimates and measured values of specific heats from **Table 5** were used to create a dataset necessary for performing mold-filling simulations.

The thermal conductivity of the AIN feedstock was estimated using **Equation 5** as a function of temperature for the 18 data points of filler specific heats (230 ± 70 W/m.K) [21], [24], [26], [30]–[32], [37]–[40]. Estimations were made for the wax-polymer binder thermal conductivity reported for temperature between 310 and 440 K. The thermal conductivity values of the wax-polymer binder used for this estimation ranged between 0.162 and 0.195 W/m.K and details for the estimation procedure are reported elsewhere [17–19, 33]. The experimentally measured and estimated values of thermal conductivity for the AIN feedstock are presented in **Table 6**. The average values of thermal conductivity estimates and measured values of thermal conductivity from **Table 6** were used to create a dataset necessary for performing mold-filling simulations.

In the present study, a simplified Krieger-Dougherty model (**Equation 6**) was used to estimate viscosity. The viscosity of the AIN feedstock was estimated for 40 different shear rates in ranges between 10 and 10^4 s⁻¹ and for temperatures of 415, 420, 425 and 430 K using **Equation 6** and polymer binder viscosity ($\eta_{b \text{ exp}}$) values from **Figure 3**. The viscosity data for the wax-polymer binder was gathered from literature [19]. The volume fraction of the AIN feedstock (ϕ_p) was calculated to be 0.52 using **Equation 2**. Viscosity was estimated for a ϕ_{max} of 0.64 critical filler content and details for the estimation procedure are reported elsewhere [17–19, 33]. The representative values for the estimated and experimental AIN feedstock viscosities are shown in **Table 7**.

To perform mold-filling simulations the viscosity of the AIN feedstock has to be represented in terms of fitted constants. The Cross-WLF model (**Equations 7 and 8**) was used to extract fitted constants from the measured and estimated AIN feedstock viscosity (**Table 8**) and details for the extraction procedure are reported elsewhere [17–

19, 33]. The Cross-WLF constants from **Table 8** were further used to create a dataset necessary for performing mold filling simulations.

A rule-of-mixtures model (**Equation 9**) was used to estimate the specific volume of AIN feedstock. To calculate the specific volume of AIN filler, the reciprocals of the densities of the AIN filler were used. The specific volume of the AIN feedstock was estimated for 20 different temperatures in ranges between 300 and 453 K and for pressures of 0, 50, 100, 150, and 200 MPa using **Equation 9** and polymer binder specific volume ($v_{b\ exp}$) values from **Figure 4**. The specific volume data for the wax-polymer binder was gathered from literature [19]. The average value for the AIN filler specific volume was used to estimate the AIN feedstock specific volume and details for the estimation procedure are reported elsewhere [17–19, 33]. The representative values for the estimated and experimental AIN feedstock specific volumes are shown in **Table 9**.

To perform mold-filling simulations, the specific volume of the AIN feedstock needs to be represented in terms of fitted constants. A dual-domain Tait model (**Equations 10-13**) was used to extract these fitted constants for the estimated and measured AIN feedstock specific volumes (**Table 10**) and details for the extraction procedure are reported elsewhere [17–19, 33]. The Dual-domain Tait constants from **Table 10** were further used to create a dataset necessary for performing mold filling simulations.

3.1. Injection molding results

The first injection molding experiment listed in **Table 1** was performed for an injection pressure of 38 MPa and a melt temperature of 455 K with the AIN feedstock. This particular combination of injection pressure and melt temperature resulted in 100% filled parts (**Figure 1a**). Additional injection molding experiments with an increase in injection pressure to a value of 48 MPa also resulted in a 100% filled parts. This behavior indicated that an increase in injection pressure from 30 to 48 MPa showed no sensitivity towards the fraction of mold cavity that was filled with feedstock.

Injection molding experiments 2-4 listed in **Table 1** were performed at a lower injection pressure of 14 MPa and the melt temperature was decreased from 444K to 389 K.

Experiments # 2-4 were performed to investigate the sensitivity of variation in injection pressure and melt temperature towards part filling. Specimen images of molded parts for experiments # 2-4 are represented in **Figure 1b-d**. Molding experiment #2 performed at a melt temperature of 444 K resulted in a 100% filled part (**Figure 1b**). Molding experiment # 3 performed at a melt temperature of 433 K resulted in a 89 % filled part (**Figure 1c**). Molding experiment #3 performed at a melt temperature of 389 K resulted in 71 % filled part (**Figure 1d**). Thus, the onset of an incomplete mold filling (short shot) was experimentally estimated at a melt temperature of 433 K (**Figure 1c**).

The PIM simulations were performed using the AIN feedstock property datasets 1-3 presented in **Table 11**. Feedstock property dataset 1 comprises of experimentally measured physical, thermal and rheological feedstock properties. Feedstock property dataset 2 comprises of estimated physical, thermal and rheological properties. Feedstock property dataset 3 comprises of estimated physical, thermal properties, and experimentally measured rheological properties.

In order to study the effectiveness of the PIM simulations in predicting mold-filling behavior, simulations were performed for the experimental processing conditions listed in **Table 1**. **Figure 5** show a typical progressive mold-filling behavior for a PIM simulation performed at an injection pressure of 38 MPa and melt temperature of 455 K using feedstock property dataset 1. A similar progressive mold-filling behavior was observed for simulations performed with feedstock property datasets 2 and 3 at an injection pressure of 38 MPa.

Simulations performed at a lower injection pressure of 14 MPa and melt temperature of 444K using datasets 1-3 also displayed a filling profile similar to that observed in **Figure 5**. In order to study, how well PIM simulations predict the melt temperature at which the short shot occurs, the melt temperature was lowered in simulations until a short shot occurred. The simulation performed with dataset 1 resulted in complete mold fill for melt temperatures until 350 K and a short shot occurred at a melt temperature of 330 K with 89 percent mold fill (**Figure 6a**). Simulations with dataset 2 resulted in complete mold fill for melt temperatures until 430K and a short shot occurred at a melt temperature of 420K with 97 percent mold fill (**Figure 6b**). Simulations with feedstock property dataset

3 resulted in complete mold fill for melt temperatures until 353K and a short shot occurred at a melt temperature of 333K with 84 percent mold fill (**Figure 6c**).

A plot of percent mold fill with melt temperature for injection molding experiments and simulations is presented in **Figure 7**. Simulation results with feedstock property datasets 1-3 predict a complete mold fill for process input conditions set according to molding experiments #1 and #2 (**Table 1**). This behavior was also observed for the injection molding experiments. However, as the melt temperature values were lowered, the results of the onset of short shots from simulations differed from molding experiment observations.

A plot of part weight with melt temperature for injection molding experiments and simulations are presented in **Figure 8**. Part weights for injection molding experiments with complete mold fill were typically around ~9.95g and had a standard deviation of ± 0.02 . Simulations with feedstock property datasets 1-3 predict part weights with comparable accuracy for process input conditions set according to molding experiments #1 and #2 (**Table 1**). Simulations with feedstock property dataset 3 for a melt temperature of 450K showed the highest deviation of 8% in predicted part weight. However, as the melt temperature values were lowered to 389K the deviation of part weight predictions from the molding experiments increased by 31% for simulations using feedstock property dataset 2.

A plot of percent-linear shrinkage with melt temperature for injection molding experiments and simulations is presented in **Figure 9**. Percent linear shrinkages for injection molding experiments with complete mold fill were typically around 0.8% and had a standard deviation of ± 0.15 . Simulations with feedstock property datasets 1-3 predict percent linear shrinkages with comparable accuracy for process input conditions set according to molding experiments #1 and #2 (**Table 1**). For ceramic-filled polymers, the percent linear shrinkage has been reported to range between 0.4 and 0.8 % [41]. The predicted and experimental values of percent-linear shrinkage are on the same order of magnitude as observed in the limited data in the literature for ceramic feedstocks.

A plot of injection pressure and melt temperature for injection molding experiments and simulations are presented in **Figure 10**. The injection-molding experiments were conducted by setting an injection pressure to a desired value. The feedstock melt was injected at this pressure and a set flow rate of $33 \text{ cm}^3/\text{s}$. The PIM simulations also allow setting of a specific value for injection pressure and flow rate. The simulation tries to attain this injection pressure value by filling the mold cavity at the desired flow rate.

Figure 10 shows the simulated values for the maximum injection pressure that can be attained during mold filling. It can be observed from **Figure 10** that simulations with feedstock property datasets 1-3 underestimate injection pressures by a factor of 30 and 10 for process input conditions set according to molding experiments #1 and #2 respectively. (**Table 2**). For simulations performed with feedstock property dataset 2 and for process input conditions set according to molding experiments #3 and #4 (**Table 2**), the injection pressure values are close to that of the actual experiments. A cause for this sensitivity is not presently understood. In the future, simulations using a different PIM simulation software package based on alternative constitutive models will be studied.

4. Conclusions

The present study can be used as a design approach to perform PIM simulations by estimating feedstock properties and study a wide variety of material systems. The current investigation was found to have the following key attributes:

1. Literature filler properties can be used in conjunction with mixture models to estimate physical, thermal, and rheological properties of AIN feedstocks.
2. Mold-filling behavior for injection molding experiments and PIM simulations are similar for parts that showed 100% mold filling. Short shot predictions using simulations were however not in full agreement with injection-molding experiments.
3. Part weight predictions by PIM simulations melt temperature 444-455K and injection pressures of 14-38 MPa, were in agreement with molding experiments within a maximum error of 8%.

4. Percent linear shrinkages for PIM simulations ranged between 0.3-1.4% and were comparable to results from injection molding experiments that ranged between 0.65-0.95%.

5. Injection pressure predictions by simulations are very sensitive to feedstock properties and warrant further investigation using other PIM software packages.

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Table 1. Models used in present study to estimate the feedstock properties

Property	Empirical relations	#
density	$\frac{1}{\rho_c} = \frac{X_b}{\rho_{b \text{ exp}}} + \frac{X_p}{\rho_p}$	1
volume fraction	$\phi_p = \frac{X_p/\rho_p}{X_p/\rho_p + X_b/\rho_{b \text{ exp}}}$	2
	$\phi_b = \frac{X_b/\rho_b}{X_p/\rho_p + X_b/\rho_{b \text{ exp}}}$	3
specific heat	$C_{p_c} = [C_{p_{b \text{ exp}}}X_b + C_{p_p}X_p] * [1 + A * X_bX_p]$	4
thermal conductivity	$1 - \phi_p = \left(\frac{\lambda_p - \lambda_c}{\lambda_p - \lambda_{b \text{ exp}}} \right) \left(\frac{\lambda_b}{\lambda_c} \right)^{1/3}$	5
viscosity	$\eta_c = \frac{\eta_{b \text{ exp}}}{\left[1 - \frac{\phi_c}{\phi_{max}} \right]^2}$	6
	$\eta_c = \frac{\eta_0}{1 + \left(\frac{\eta_0 \gamma}{\tau^*} \right)^{1-n}}$	7
	$\eta_0 = D_1 \exp \left[-\frac{A_1(T - T^*)}{A_2 + (T - T^*)} \right]$	8
specific volume	$v_c = X_p v_p + v_{b \text{ exp}}(1 - X_p)$	9
	$v(T, p) = v_o(T) \left[1 - C \ln \left(1 + \frac{p}{B(T)} \right) + v_t(T, p) \right]$	10
	for $T > T_t$ $v_o = b_{1m} + b_{2m}(T - b_5); \quad B(T) = b_{3m}e^{[-b_{4m}(T - b_5)]};$ $v_t(T, p) = 0$	11
	for $T < T_t$; $v_o = b_{1s} + b_{2s}(T - b_5); \quad B(T) = b_{2s}e^{[-b_{4s}(T - b_5)]};$ $v_t(T, p) = b_7 e^{[b_8(T - b_5) - (b_9 p)]}$	12
	$T_t(p) = b_5 + b_6(p)$	13

Table 2. Description of symbols used in the paper

Symbol	Description
T_m	melt temperature
X_c	mass fraction of feedstock
X_b	mass fraction of binder
X_p	mass fraction of filler
ρ_c	density of feedstock
ρ_b	measured density of binder
ρ_p	density of filler
$\rho_{c\ est}$	estimated average density of feedstock
$C_{p\ c}$	specific heat of feedstock
$C_{p\ b\ exp}$	measured specific heat of binder
$C_{p\ p}$	specific heat of filler
A	=0.2 fitting constant for spherical powders
$C_{p\ c\ est}$	estimated average specific heat of feedstock
λ_c	thermal conductivity of feedstock
$\lambda_{b\ exp}$	measured thermal conductivity of binder
λ_p	thermal conductivity of filler
$\lambda_{c\ est}$	estimated average thermal conductivity of feedstock
ϕ_c	volume fraction of feedstock
ϕ_b	volume fraction of binder
ϕ_p	volume fraction of filler

Table 2 Continued. Description of symbols used in the paper

symbol	description
$\eta_{b \text{ exp}}$	viscosity of binder
η_c	viscosity of feedstock
ϕ_{max}	(0.64) volume fraction of critical solids loading of feedstock
$\eta_{c \text{ est}}$	estimated average viscosity of feedstock at $\phi_{max}=0.64$
η_0	is the zero shear viscosity
γ	shear rate
τ^*	critical stress level at the transition to shear thinning determined by curve fitting
n	power law index in the high shear rate regime
T	temperature
$T^* D_1 \text{ and } A_1$	curve fitted coefficients
A_2	(51.6 K) WLF constant
v_c	specific volume of feedstock
$v_{b \text{ exp}}$	measured specific volume of binder
v_p	specific volume of filler
$v_{c \text{ est}}$	estimated average specific volume of feedstock
$v(T, p)$	specific volume at a given temperature and pressure
v_0	specific volume at zero gauge pressure
p	pressure
C	(0.0894) constant
$b_{1s} b_{2s} b_{3s} b_{4s}$ $b_5 b_7 b_8 \text{ and } b_9$	curve-fitted coefficients
$b_{1m} b_{2m} b_{3m}$ $b_{4m} b_5 \text{ and } b_6$	curve-fitted coefficients
$B(T)$	pressure sensitivity material as a function of temperature

Table 3. Molding parameters for AIN tensile bar geometry

molding parameters	experiment number, #			
	# 1	# 2	# 3	# 4
mold temperature, K	297	297	297	297
melt temperature, K	455	444	433	422
injection speed, cm ³ /s	33	33	33	33
injection pressure, MPa	38	14	14	14
packing pressure 1, MPa for 1 s	38	14	14	14
packing pressure 2, MPa for 1.2 s	25	9	9	9

*variation in temperature profile; **variation in pressure profile

Table 4. Density of the AIN feedstock and wax-polymer binder at 300 K

Density, m ³ /kg	$\rho_{c \text{ exp}}^*$	$\rho_{c \text{ est}}^+$
solid	2150	2130±20
melt	1940	1940±20

*measured experimentally; +estimated using **Equation 4.1** for 22 data points of ρ_p

Table 5. Specific heat of the AIN feedstock and wax-polymer binder for temperature between 283 and 423 K

specific heat C_p , J/kg-K	Temperature, K				
	283	298	331	374	423
$C_{p \text{ exp}}^*$	920	1110	1090	1130	1210
$C_{p \text{ est}}^+$	1050±35	1240±35	1570±35	1850±35	1150±35

*measured experimentally; +estimated using **Equation 4.4** for 6 data points of C_{p_p}

Table 6. Thermal conductivity of AlN feedstock and wax-polymer binder for temperature between 316 and 436 K

thermal conductivity, W/m-K	temperature, K				
	316	356	377	397	436
$\lambda_{c \text{ exp}}^*$	4.26	2.23	2.66	2.06	2.50
$\lambda_{c \text{ est}}^+$	1.82 ± 0.01	1.71 ± 0.01	1.67 ± 0.06	1.62 ± 0.08	1.55 ± 0.10

*measured experimentally; +estimated using **Equation 4.5** for 18 data points of λ_p

Table 7. Viscosity of the AlN feedstock as a function of shear rate between 10^1 and 10^4 s⁻¹ for a temperature range of 415 to 430 K

shear rate s ⁻¹	viscosity η_c , Pa.s @ $\phi_{max} = 0.64$					
	T = 415 K		T = 425 K		T = 430 K	
	$\eta_{c \text{ exp}}^*$	$\eta_{c \text{ est}}^+$	$\eta_{c \text{ exp}}^*$	$\eta_{c \text{ est}}^+$	$\eta_{c \text{ exp}}^*$	$\eta_{c \text{ est}}^+$
10^1	1470	4830	1380	1330	1340	660
10^2	350	1460	330	540	320	890
10^3	80	390	80	160	80	100
10^4	20	100	20	40	20	30

*measured experimentally; +estimated using **Equation 6**

Table 8. Cross-WLF constants for the AlN feedstock

Cross WLF constants	$\eta_{c \text{ exp}}^*$	$\eta_{c \text{ est}}^+$
n	0.38	0.40
τ^* , Pa	180	26860
D ₁ , Pa.s	8.78X10¹⁰	2.23X10 ¹⁵
D ₂ , K	263	360.93
A ₁ , K/Pa	14.24	49.55
A ₂ , K	51.60	51.60

*calculated from **Equation 7, 8** and experimental (η_c) values from **Table 7**;

+calculated from **Equation 7, 8** and estimated (η_c) values from **Table 7**

Table 9. Specific volume of the AlN feedstock as a function of pressure between 0 MPa and 200 MPa for a temperature range of 300 to 450 K

Temperature, K	specific volume $\times 10^{-3}$, m ³ /kg					
	P = 0 MPa		P = 100 MPa		P = 200 MPa	
	$v_{c \text{ exp}}^*$	$v_{c \text{ est}}^+$	$v_{c \text{ exp}}^*$	$v_{c \text{ est}}^+$	$v_{c \text{ exp}}$	$v_{c \text{ est}}^+$
300	0.47	0.48	0.46	0.47	0.45	0.46
350	0.49	0.50	0.48	0.49	0.46	0.47
400	0.50	0.51	0.49	0.50	0.47	0.49
450	0.52	0.53	0.50	0.50	0.48	0.49

*measured experimentally; +estimated using **Equation 9**

Table 10. Dual-domain Tait constants for the AlN feedstock

Dual-domain Tait constants	$v_{c \text{ exp}}^*$	$v_{c \text{ est}}^+$
b_5 , K	331	331
b_6 , K/Pa	1.30×10^{-7}	1.30×10^{-7}
b_{1m} , m ³ /kg	4.64×10^{-4}	5.77×10^{-4}
b_{2m} , m ³ /kg.K	1.87×10^{-7}	1.95×10^{-7}
b_{3m} , Pa	2.05×10^9	2.17×10^9
b_{4m} , 1/K	4.60×10^{-3}	6.15×10^{-3}
b_{1s} , m ³ /kg	4.55×10^{-4}	5.69×10^{-4}
b_{2s} , m ³ /kg.K	2.05×10^{-7}	2.05×10^{-7}
b_{3s} , Pa	2.52×10^9	1.63×10^9
b_{4s} , 1/K	3.01×10^{-3}	6.35×10^{-3}
b_7 , m ³ /kg	5.08×10^{-5}	5.34×10^{-5}
b_8 , 1/K	8.54×10^{-1}	8.97×10^{-1}
b_9 , 1/Pa	5.06×10^{-6}	3.53×10^{-5}

*calculated from **Equation 10-13** and experimental (v_c) values from **Table 9**;

+calculated from **Equation 1-13** and estimated (v_c) values from **Table 9**

Table 11. AIN feedstock property datasets used for injection molding simulations

AIN feedstock dataset	density* ρ_c , kg/m ³	specific heat** C_{p_c} , J/kg-K	thermal conductivity+ λ_c , W/m-K	Cross WLF constants++	Dual-domain Tait constants*+
1	$\rho_{c \text{ exp}}$	$C_{p_c \text{ exp}}$	$\lambda_{c \text{ exp}}$	$\eta_{c \text{ exp}}$	$\nu_{c \text{ exp}}$
2	$\rho_{c \text{ est}}$	$C_{p_c \text{ est}}$	$\lambda_{c \text{ est}}$	$\eta_{c \text{ est}}$	$\nu_{c \text{ est}}$
3	$\rho_{c \text{ est}}$	$C_{p_c \text{ est}}$	$\lambda_{c \text{ est}}$	$\eta_{c \text{ exp}}$	$\nu_{c \text{ est}}$

*data from **Table 4**; **data from **Table 5**; +data from **Table 6**;

++data from **Table 8**; and +*data from **Table 10**