

# Modélisation et analyse de processus pour l'écriture directe à l'encre basée sur des simulations numériques Yongqiang Tu

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## ÉCOLE DOCTORALE SCIENCES DES MÉTIERS DE L'INGÉNIEUR [Laboratoire de Conception, Fabrication, Commande – Campus de Metz]

# THÈSE

# pr ésent ée par: Yongqiang TU

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Sp écialit é G énie industriel

# Process modeling and analysis for direct ink writing based on numerical simulations

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Nomenclature

AM	Additive manufacturing
ANOVA	Analysis of variance
BJ	Binder jetting
BJ3DP	Binder jet 3D printing
CAD	Computer-aided design
CFD	Computational fluid dynamics
DED	Directed energy deposition
DF	Deposited filament
DIW	Direct ink writing
DLP	Digital light processing
DMD	Digital micro-mirror device
DMLS	Direct metal laser sintering
DOE	Design of experiments
DOF	Design of freedom
EBM	Electron beam melting
FDM	Fused deposition modeling
FEA	Finite element analysis
FEF	Freeform extruded filament
HBM	Hershel-Bulkley model
IJP	Inkjet printing
LOM	Laminated object manufacturing
MDDSEO	Maximum distance deviation between simulated and
MF	Material extrusion
MEAM	Material extrusion AM
MI	Material jetting
МІ	Machine learning
	waching learning

OA	Orthogonal array
PBDED	Powder based directed energy deposition
PBF	Powder bed fusion
PLA	Poly-lactic acid
RSM	Response surface methodology
SHL	Sheet lamination
SHS	Selective heat sintering
SL	Stereolithography
SLM	Selective laser melting
SLS	Selective laser sintering
SNR	Signal-to-noise ratio
TPP	Two-photon polymerization
UV	Ultraviolet
VOF	Volume of fluid
VPP	Vat photo polymerization
WBDED	Wire based directed energy deposition
2D	Two-dimensional
3D	Three-dimensional
G'	Storage modulus
G"	Loss modulus
τ	Shear stress
<i>3</i> &	Shear rate
μ	Viscosity of the ink
$\mu_{0}$	Limiting dynamic viscosity
$ au_0$	Yield stress
Κ	Consistency index
n	Flow index
$\theta_{c}$	Static contact angle

$R^2$	Coefficient of determination
ρ	Density of the ink
σ	Surface tension coefficient
$D_p$	Piston diameter
$d_n$	Inner diameter of nozzle
$D_n$	Outer diameter of nozzle
$L_n$	Nozzle length
$L_0$	Initial filled length of ink
h	Distance between nozzle bottom and substrate
V <sub>e</sub>	Average velocity of ink in nozzle
V <sub>p</sub>	Piston velocity
V <sub>n</sub>	Nozzle velocity
$V^*$	Dimensionless nozzle velocity, $= v_n / v_e$
$H^*$	Dimensionless height, $= h / d_n$
$\overline{w}_o$	Average width of the optimal printed line
$d_{i}$	Distance between lines
$R_w$	Ratio of $d_i$ to $\overline{w}_o$
W	Weight of the printed layer
$N_1$	Number of measuring points set along the line length
$w_i (i = 1, 2,, N_1)$	Widths of line on each measuring point
$\overline{w}$	Average width of printed line
$el_i(i = 1, 2,, N_1)$	Dimensional errors on each measuring point along length
$N_2$	Number of measuring points set along x direction in printed rectangular object
N <sub>3</sub>	Number of measuring points set along y direction in printed rectangular object

$lx_i (i = 1, 2,, N_2)$	Lengths on each measuring point along x direction of printed rectangular object
$ly_i (i = 1, 2,, N_3)$	Lengths on each measuring point along y direction of printed rectangular object
<i>lx</i>	Average length in x direction of printed rectangular object
$\overline{l}y$	Average length in y direction of printed rectangular object
Lx	Designed dimension for rectangular object in x direction
Ly	Designed dimension for rectangular object in y direction
$erx_i (i = 1, 2,, N_2)$	Dimensional error for the printed rectangular object in x directions
$ery_i (i = 1, 2,, N_3)$	Dimensional error for the printed rectangular object in y directions
S	DOF of a factor
Т	Number of experiments
DOF <sub>total</sub>	Total DOF of factors and their interaction effects
$L_{T}$	OA with $T$ experiments
η	Average SNR
α	Phase fraction for a mesh
$V_i$	Volume of the ink in a mesh
$V_m$	Total volume of a mesh
$ ho_s$	Density of the single continuum
$\mu_s$	Viscosity of the single continuum
$ ho_a$	Density of the air
$\mu_a$	Viscosity of the air
U	Velocity field
p	Pressure
g	Gravitational acceleration vector
$\mathbf{F}_{\sigma}$	Surface tension

κ	Surface curvature
n	Normal vector to the ink surface
n	Unit vector normal to the ink surface
$\hat{\mathbf{n}}_{w}$	Unit vector normal to the substrate
$\hat{\mathbf{t}}_{w}$	Unit vector tangent to the substrate
t	Time
U <sub>r</sub>	Velocity vector compressing two-phase free surface
С	Controllable compression factor
$E_{f}$	Diameter prediction accuracy of numerical simulation of FEF
$N_{_f}$	Number of measurement points in FEF
e <sub>fi</sub>	Diameter difference between experimental and simulation results
$d_{fi}$	Diameter of FEF
β	Ratio of $D_n$ to $d_n$ , $= D_n / d_n$
γ	$= \left(\theta_c - \frac{\sin 2\theta_c}{2}\right) \left(\frac{1}{1 - \cos \theta_c}\right)^2$
$h_{d}$	Height of DF
w <sub>d</sub>	Width of DF
θ	Angle of deposited corners
v <sub>n1</sub>	Nozzle velocity on substrate 1
v <sub>n2</sub>	Nozzle velocity on substrate 2
V <sub>nx</sub>	Velocity on substrate along x axis
V <sub>ny</sub>	Velocity on substrate along y axis

R ésum é Étendu En Fran çais

#### **1** Introduction générale

#### 1.1 Contexte et objectif de la thèse

La fabrication additive (FA) est une technologie de fabrication avanc é qui imprime directement des pi èces tridimensionnelles (3D) en empilant des mat ériaux couche par couche sur la base d'un mod de num érique 3D de conception assist ée par ordinateur (CAO) [1-5]. Par rapport aux techniques de fabrication traditionnelles telles que le forgeage, le moulage, le soudage et l'usinage (tournage, fraisage, rabotage, meulage, etc.), la FA pr ésente les avantages de la num érisation, de l'économie de mati ère, de la diversification des mat ériaux et de la possibilit é de fabriquer facilement des pi èces complexes, qui r épondent les exigences de haute pr écision, de libert é structurelle et de personnalisation pour le d éveloppement de nouveaux mat ériaux et de nouvelles structures dans l'ing énierie tissulaire, la m édecine, l'ing énierie du caoutchouc, l'ing énierie c éramique, les capteurs, l'aviation, l'a érospatiale, l'éctronique, l'alimentation et d'autres applications industrielles [6-10]. Selon ISO/ASTM 52900 (2015), la fabrication additive est divis é en sept cat égories bas ées sur le principe de fonctionnement : jet de liant (BJ), d ép ât d'énergie dirig é (DED), extrusion de mat ériau (ME), jet de mat ériau (MJ), fusion sur lit de poudre (PBF), laminage de feuilles (SHL) et photopolym érisation en cuve (VPP).

L'ériture directe à l'encre (DIW) appartient à l'extrusion de mat ériau (MEAM) selon le principe de fonctionnement. Le principe de fonctionnement de DIW est le suivant : premi àrement, le mat ériau est pr épar é sous forme de p âte ou de suspension avec une bonne imprimabilit é appel ée encre ; puis l'encre est extrud ée àpartir d'une buse en filaments continus à l'aide d'une force m écanique (piston ou entra înement par vis) ou d'une force pneumatique ; et enfin les filaments sont d épos és en parties 3D par couches [11]. Par rapport àd'autres techniques de la FA, DIW pr ésente les avantages exceptionnels de la diversit é des mat ériaux et de la flexibilit é des équipements [12-14]. En raison de ses avantages, DIW est devenu l'une des techniques FA les plus populaires ces derni àres ann ées.

Cependant, la compr énension et l'analyse du processus de DIW n'ont pas étéenti èrement étudi ées, ce qui limite la précision de fabrication et la promotion de l'application de cette technique. Dans des études récentes, en raison du manque de compr énension et d'analyse des processus de DIW, les chercheurs doivent passer par de nombreux essais pour trouver une fen être imprimable des propri étés de l'encre et des param ètres de processus adapt és au DIW pour obtenir la qualit é d'impression qui répond aux exigences d'utilisation [15-17], ce qui augmente consid érablement les coûts et réduit l'attractivit é des applications de DIW. Pour r ésoudre ce problème, il est essentiel de faire des recherches sur l'analyse des processus pour DIW afin de bien comprendre ce processus et d'am diorer la convivialit éde DIW. La simulation num érique est l'un des outils les plus puissants d'analyse de processus en AM. L'analyse de processus bas ée sur des simulations num ériques pr ésente des avantages en termes d'économie de temps de mat ériau/d'essai et de capture facile de la valeur des param ètres de processus critiques qui sont difficiles à obtenir par des mesures expérimentales. La recherche sur la mod disation des processus et l'analyse de DIW bas ée sur des simulations num ériques fournira un soutien important pour le développement et l'orientation de DIW. Cependant, il existe actuellement peu de travaux syst ématiques sur la mod disation et l'analyse des processus bas és sur des simulations num ériques pour DIW. Pour combler cette lacune, l'objectif de cette th èse est de contribuer àla mod disation et àl'analyse des processus DIW bas ées sur des simulations num ériques.

#### 1.2 Contenu de la recherche

Le processus DIW est influenc é à la fois par les propri é és du mat ériau de l'encre et les param ètres du processus. Les propri é és des mat ériaux d'encre et les param ètres de processus sont des conditions d'entr ée dans les simulations num ériques. Ainsi, une fois la caract érisation des propri é és des mat ériaux d'encre et la s élection des param ètres de processus sont étudi ées, les r ésultats de la recherche sont utilis és comme conditions d'entr ée pour les simulations num ériques. Ensuite, des simulations num ériques pour DIW sont r éalis ées. En tant que l'une des technologies FA, comme le montre la figure 1.1, l'ensemble des étapes du processus de DIW comprend :

- Étape 1 : Mod disation g éom étrique 3D àl'aide d'une conception descendante dans un logiciel de mod disation 3D comme Solidworks, ProE, UG, CATIA, 3DMAx, etc. ou en utilisant une conception d'inversion bas ée sur les donn ées du mod de 3D de la technologie de r éalit é virtuelle ou du scanner 3D ;
- Étape 2 : G én ération de G-code en important le format STL du mod de g éom érique
   3D et en d éfinissant les param ètres de processus dans le logiciel Slicer ;
- Étape 3 : Impression dans une imprimante 3D DIW àl'aide du G-code g én ér évia le processus de fabrication par couches.

En particulier, DIW peut imprimer des pi àces 3D arbitrairement complexes par extrusion d'encre, points àligne, lignes àcouche et couches àpi àces 3D, comme illustr é dans le tableau de l'étape 3 de la figure 1.1. Parmi ce processus, le filament extrud é de forme libre (FEF), le filament d'épos é (DF) et le coin d'épos é sont les éléments les plus fondamentaux et les plus

critiques. Ainsi, la thèse porte sur les simulations num ériques et les analyses de processus de ces él éments fondamentaux et critiques : FEF, DF et coin d'épos é

En conclusion, pour atteindre l'objectif de la thèse, le contenu de la recherche comprend :

- Recherche sur la caract érisation des propri ét és des mat ériaux d'encre et la s élection des param ètres de processus ;
- Recherche sur la simulation num 

  érique des 

  é éments de base et critiques dans DIW,
  y compris FEF, DF et coin d 

  épos 

  é;
- V érifications exp érimentales des simulations num ériques propos éss ;
- Analyse de processus bas é sur les simulations num ériques propos és.



Figure 1.1 Illustration du processus de DIW et l'objetif de recherche r ésum é dans cette th èse : (a) mod èle CAO construit dans un logiciel de mod élisation 3D ; (b) Mod èle CAO à partir d'un scanner 3D ; (c) Mod èle CAO enregistr é au format STL ; (d) Mod èle 3D import é dans le logiciel Slicer ; (e) r églage des param ètres de processus dans le logiciel Slicer ; (f) Gcode g én ér é à l'aide du logiciel Slicer ; (g) composition m écanique de l'imprimante 3D DIW ;

(h) encre dans la seringue ; (i) photo r éelle de l'imprimante 3D DIW ; (j) processus
d'extrusion d'encre; (k) processus point àligne ; (l) processus lignes-couches ; (m) processus
de pi èces en couches en 3D ; (n) é énents de base et critiques du processus DIW ; (o) objetif
de recherche r ésum é

#### **1.3** Structure de la thèse

Cette thèse est structur ée en cinq chapitres et le contenu de chaque chapitre est bri èvement introduit comme suit :

Le chapitre 1 donne un aper çu du contexte et de l'objectif de la recherche. Enfin, la structure de la thèse est esquiss é.

Le chapitre 2 pr ésente l' état de l'art, une revue syst ématique de la litt érature de DIW est men ét d'abord pour r ésumer les caract éristiques, le d éveloppement, les d éfis et les solutions aux d éfis de DIW et un problème insuffisamment r ésolu est d étermin é comme la question de recherche de cette thèse. Pour r épondre àla la question de recherche, la mod élisation et l'analyse des processus pour DIW sont s électionn és afin d'apporter une réponse. Ensuite, une litt érature sur la mod élisation et l'analyse des processus pour DIW est r éalis ét. Les entr és et les sorties de la mod élisation de processus de DIW sont r ésum és et les méthodes de mod élisation de processus num ériques sont s électionn és comme la méthode la plus appropri ét pour la mod élisation de processus et l'analyse de DIW. Enfin, l'objectif de cette thèse est repositionn é par rapport àla revue de la litt érature.

Le chapitre 3 présente les travaux sur la caract érisation des propri étés des mat ériaux d'encre et la s dection des param àres de processus pour fournir les entr ées de la mod disation. Pour la caract érisation des propri étés du mat ériau de l'encre, la densit é, la tension superficielle, l'angle de contact statique et les propri étés rh éologiques sont obtenues pour l'encre utilis ée. Pour la s dection des param àres de processus, les param àres de processus DIW sont identifi és par des analyses d'impression via un plan d'expérience. Ainsi, une m éthode d'optimisation en deux étapes est propos ée pour optimiser les param àres de processus DIW pour la précision dimensionnelle des couches imprim ées et l'analyse de l'importance de chaque param àre de processus.

Le chapitre 4 pr ésente les simulations num ériques de FEF, DF et des coins d épos és dans DIW. Dans un premier temps, la m éhode de simulation num érique, volume de fluide (VOF), est introduite. Ensuite, des simulations num ériques de FEF, DF et des coins d épos és sont pr ésent és à travers la mod élisation g éom érique, la g én ération de maillages, la d étermination des conditions aux limites. Ensuite, des v érifications exp érimentales sont men és pour v érifier les simulations num ériques propos és. Enfin, l'analyse du processus est effectu ée sur la base du mod è de simulation num érique propos é

Le chapitre 5 pr ésente la conclusion et les perspectives de la thèse.

# 2 État de l'art

#### 2.1 Introduction

Ces derni ères ann és, DIW a attir éune grande attention à la fois du milieu universitaire et de l'industrie, et DIW est devenu l'une des techniques FA les plus populaires. Cependant, en tant que technique qui s'est d'évelopp ér rapidement ces derni ères ann és, il reste encore de nombreux probl èmes à r ésoudre dans l'utilisation pratique de DIW et un état de l'art complet de DIW est essentiel pour comprendre son statut de d'éveloppement et ses probl èmes. Un état de l'art de la technique DIW a été d'abord mené et les problèmes potentiels liés à celle-ci ont été identifiés. Les résultats de l'état de l'art ont conclu à la mod étisation et l'analyse des processus DIW à l'aide de simulations num ériques sont comme un moyen efficace de r ésoudre les probl èmes non r ésolus. Ainsi, une revue de la litt érature sur la mod étisation et l'analyse des processus à l'aide de simulations num ériques pour DIW est en outre effectu ée et les lacunes de la recherche sont r ésou.

Le reste de ce chapitre est organis é comme suit. La section 2.2 présente la revue syst ématique de la litt érature sur DIW. Elle présente d'abord la criticit é de la technologie FA dans la section 2.2.1. Ensuite, les techniques FA les plus couramment utilis és sont présent és et les caract éristiques de chaque technique FA sont r ésum és pour analyser les avantages et les applications appropri és de DIW dans la section 2.2.2. Ensuite, le d'éveloppement, les d'éfis et les solutions existantes de DIW sont examin és et la question de recherche de cette th èse dans la section 2.2.3 a ét é formul é. Pour r ésoudre la question de recherche, la mod élisation et l'analyse des processus pour DIW sont s dectionn és comme base de solution. Ainsi, la mod élisation et l'analyse des processus pour DIW sont examin és dans la section 2.3.1 et les entr és et les sorties de la mod élisation des processus sont r ésum és dans la section 2.3.2. Sur la base des

lacunes de la recherche r ésum és dans la revue de la litt érature, la section 2.3.3 identifie l'objectif de cette th èse.

#### 2.2 Une revue de la litt érature sur DIW

Au cours des cinq derni ères ann és, la technologie FA a suscit é une grande attention et a ét é utilis ée avec succ ès dans diverses applications présentant un grand potentiel commercial (Figure 2.1). Et comme le montre la Figure 2.2, les techniques de fabrication additive couramment utilis ées comprennent : l'impression 3D par jet de liant (BJ3DP), la fabrication d'objets lamin és (LOM), la mod élisation par dépôt de fil fondu (FDM), l'ériture directe à l'encre (DIW), l'impression àjet d'encre (IJP), l'impression s élective frittage laser (SLS), fusion laser s élective (SLM), dépôt d'énergie dirigée à base de poudre (PBDED), dépôt d'énergie dirigée à base de fil (WBDED), st ér éolithographie (SL), traitement num érique de la lumi ère (DLP) et polym érisation àdeux photons (TPP).



Figure 2.1 (a) Applications de la FA et part de production dans divers secteurs et (b) Production annuelle de pi èces FA par des fournisseurs de services ind épendants dans le monde entier (en millions de dollars am éricains) [24]



Figure 2.2 Classification et illustrations de différentes techniques FA couramment utilisées : (a) BJ3DP, (b) LOM, (c) FDM, (d) DIW, (e) IJP, (f) SLS/SLM, (g) PBDED, (h) WBDED, (i) SL, (j) DLP, (k) TTP

Les caract éristiques de chaque technique FA sont r ésum és dans le tableau 2.1 [24] :

Technique FM	Caract <del>é</del> ristiques	Mat <del>ér</del> iaux applicables	Forme de la mati <del>è</del> re	M <del>á</del> thode de formage	Exigence d'impression	R ésolution
BJ3DP	R ésistance limit ée et surfaces rugueuses	M  áaux, sable, c  áamique	Lisier & Poudre	Collage de liant	Besoin d'un liant	µm àmm
LOM	Faible vitesse et grande taille, faible pr écision, limit épar le liant	Papier, plastique, m <del>d</del> aux, c <del>c</del> amique	Laminage	Empilage et d écoupe laser	Laminage	mm
FDM	Vitesse dev é et grande taille, faible pr écision, limit é par la temp érature d'extrusion	Polym ères thermoplastiques	Filament	Extrusion	A l' <del>c</del> tat de filament	mm
DIW	Grande vitesse, faible co ût, large choix de mat ériaux	Polym àres, bio- encre, m átaux, ciment, c áramique	Encrer	Extrusion	Viscosit éet propri	Quelques 100 µm à mm
IJP	Moins de quantit é de mati àre, limit ée par les encres imprimables, faible vitesse d'impression	Polymères, bio- encre, métaux, céramiques	Encrer	Formation de gouttelettes	Faible viscositéavec collage rapide	Quelques 100 µm à mm
SLS	Vitesse lente, pr cision dimensionnelle dev ce	Nylon, m <del>á</del> aux	Poudre	Frittage de poudre	Fusible au laser	µm à mm
SLM	Vitesse lente, pr écision dimensionnelle dev ée	M đaux	Poudre	Fusion de poudre	Fusible au laser	µm à mm
PBDED	Grande vitesse, grande taille	M <i>é</i> taux	Poudre	Fusion de poudre	Fondant par énergie	µm à mm
WBDED	Haute vitesse, grande taille, faible pr écision	M <del>á</del> aux	Fil	Fusion de fil	Fondant par énergie	mm
SL	Vitesse mod ér ée, rendement dev é, bonne qualit é de surface	R ésines, c éramiques	Bouillie	Polym érisation lin éaire	Photodurcissables aux UV	Sous 100 µm
DLP	Haute vitesse, rendement dev é, bonne qualit é de surface	R ésines, c éramiques	Bouillie	Polym <del>á</del> risation lin éaire	Photodurcissables aux UV	Sous 100 µm
TPP	Slow speed, high cost, fine surface quality, highest printing precision	R ésines, c éramiques	Bouillie	Polym <del>á</del> risation non lin éaire	Photopolym <del>á</del> risation àdeux photons	Sous µm

Table 2.1	Caract éristiques,	mat ériaux a	pplicables,	forme de	e la mati	ère, m	éthode d	de formage,
	exigence d'im	pression et a	r ésolution d	e chaque	techniq	ue FA	[24]	

Selon le tableau 2.1, les comparaisons de la diversit édes mat ériaux, du coût, de la vitesse, de la résolution de chaque technique FA sont répertori és comme suit:

(1) Diversit é des mat ériaux

#### <u>**DIW</u>**> IJP>LOM>BJ3DP>FDM>SL, DLP, TPP>SLS>SLM, PBDED, WBDED</u>

(2) Co ût

#### SLM>SLS>PBDED>WBDED>TPP>SL>DLP>IJP>BJ3DP>LOM>FDM>DIW

(3) Vitesse

 $IJP, \ BJ3DP > DLP > LOM > \underline{DIW} > FDM > WBDED > PBDED > SLM > SLS > SL > TPP$ 

(4) R ésolution

#### TPP>SL>DLP>SLM>SLS>PBDED>IJP>BJ3DP><u>DIW</u>>FDM>WBDED>LOM

En raison des avantages exceptionnels de la diversit édes mat ériaux et de la flexibilit édes équipements, DIW est devenu l'une des techniques AM les plus populaires et les chercheurs ont effectu é de nombreux travaux sur DIW pour la promotion de son application. Le DIW a ét é utilis éavec succ ès dans l'ing énierie du caoutchouc [62], l'ing énierie tissulaire [63], les batteries [64], les circuits dectroniques [65], les b âtiments [66], l'ing énierie c éramique [67], les capteurs et l'impression 4D [68] (Figure 2.3). Pr évisible que de plus en plus de nouveaux mat ériaux seront pr épar és sous forme d'encres adapt ées au DIW et appliqu és dans un plus grand nombre d'applications n écessitant des mat ériaux ou des pi èces structurels ou fonctionnels.

#### R ésum é étendu en français



Figure 2.3 Mat ériaux appropri és et applications correspondantes au DIW : (a) encre polym ère dans l'ing énierie du caoutchouc [62] ; (b) encre biologique dans le g énie tissulaire [63];(c) encre m étallique dans les batteries [64], circuits électroniques [65]; d) encre de ciment dans les b âtiments [66] ; e) encre c éramique dans l'ing énierie c éramique [67] ; (f) encre fonctionnelle dans l'impression 4D et les capteurs [68]

En tant que technique qui s'est d évelopp é rapidement ces derni à es ann és, bien que de nombreux chercheurs aient effectu é de nombreuses recherches sur le d éveloppement du DIW, de nombreux d éfis doivent encore être relev és pour am éliorer la finition de surface lisse, la pr écision dimensionnelle et les propri ét és (m écaniques et fonctionnelles) pour la promotion et l'industrialisation du DIW. Les principaux probl èmes de DIW sont r ésum és comme suit [9] :

(1) Difficult é àconstruire de grands surplombs ou port és avec une pr écision g éom érique parfaite malgr él'utilisation d'encre àrh éologie optimis é ;

 (2) Difficult éde pr éparation de l'encre avec une rh éologie optimis é : l'encre doit s' écouler facilement sous contrainte de cisaillement et r écup érer et conserver rapidement sa forme lors du d ép ôt ;

(3) Difficult é à extruder l'encre à travers des pi àces extrêmement petites pour imprimer des pi àces à haute r ésolution en raison du colmatage ;

(4) Difficult é à trouver rapidement des param dres de processus appropri és pour l'encre prépar ée.

De nombreux chercheurs ont effectu é diverses recherches pour proposer des suggestions et des r éf érences pour r ésoudre les problèmes. Les solutions aux problèmes ci-dessus propos és par les chercheurs sont r ésum és comme suit :

(1) Pour la question (1), les chercheurs ont utilis é des supports sacrificiels pour d'argir la gamme de g éom étries pouvant être fabriqu ées par le DIW [90] ;

(2) Pour la question (2), la question de la recherche et de nombreux travaux sur DIW se concentrent principalement sur la préparation de l'encre, puis ils s dectionnent la meilleure encre en utilisant la caractérisation rhéologique à l'aide de tests de rhéologie, y compris le test de rampe de contrainte de cisaillement, le test de balayage du taux de cisaillement, le balayage de fréquence test et test de récupération [67] ;

(3) La question (3) peut être évit ét en utilisant un lubrifiant de surface appropri étel que l'acide ol éque pour r éduire le frottement entre les particules et la formation d'agglom ération
[91] et en am éliorant la conception des buses [92] ;

(4) Les chercheurs doivent passer par de nombreux essais pour trouver une fen être imprimable de propri ét és d'encre et de param ètres de processus adapt és au DIW pour obtenir la qualit é d'impression qui r épond aux exigences d'utilisation [15-17].

La raison principale de la question (4) est que la recherche sur l'analyse du proc éd é DIW fait très d'éfaut car la mod élisation et l'analyse du proc éd é DIW n'ont pas ét é entièrement étudiées, ce qui limite la précision de fabrication et la promotion de l'application de cette technique. Cette question augmente considérablement les coûts et réduit l'attractivité des applications de DIW. Pour résoudre ce problème, il est essentiel de proposer des méhodes et des outils afin de réduire le nombre d'essais sur les encres. La mod élisation et l'analyse num ériques des processus DIW peuvent apporter une réponse àcette question.

# 2.3 Une revue de la littérature sur la modélisation et l'analyse des processus DIW

Le but de la mod disation de processus DIW est de construire la relation entre l'entr é et la sortie dans le processus d'impression 3D, qui est utilis é pour pr édire la sortie en fonction de l'entr é avant l'impression. La revue de la litt érature r ésume les entr és et les sorties de la mod disation pour DIW comme le montre la Figure 2.8. Les entr és sont les propri é és mat érielles de l'encre et le r églage des param ètres du processus d'impression. Les sorties incluent le FEF, le DF, le coin d épos é, la couche imprim é et la pi èce 3D (Figure 2.9).



Figure 2.8 Entr ées et sorties de la mod disation de processus DIW



Figure 2.9 Photos physiques des sorties de la mod disation de processus pour DIW : (a) FEF, (b) DF, (c) coin d épos é, (d) couche imprim ée, (e) pi èce 3D

La simulation num érique est l'un des outils les plus puissants d'analyse de processus en FA. L'analyse de processus bas é sur des simulations num ériques présente des avantages en termes d'économie de temps de mat ériau/d'essai et de capture facile de la valeur des param ères de processus critiques qui sont difficiles àobtenir par des mesures exp érimentales. La recherche sur la mod élisation des processus et l'analyse de DIW bas é sur des simulations num ériques fournira un soutien important pour le développement et l'orientation de DIW. Cependant, il existe actuellement peu de travaux syst ématiques sur la mod élisation et l'analyse des processus bas és sur des simulations num ériques pour DIW. Pour combler cette lacune, l'objectif de cette thèse est de contribuer à la mod élisation et l'analyse des processus DIW bas és sur des simulations num ériques.

# **3** Caractérisation des propriétés des matériaux d'encre et sélection des paramètres de traitement

La qualit éd'impression du processus DIW d épend des propri ét és du mat ériau de l'encre et du r églage des param ètres du processus. Des études r écentes [93-95] se sont concentr és sur la pr éparation des encres et la caract érisation des propri ét és des mat ériaux d'encre, car les
propri ét és des mat ériaux d'encre jouent le r de le plus critique dans le processus d'extrusion, le retrait, la fid étit éde forme et la stabilit éstructurelle. Les param ètres du proc éd éDIW concern és par l'équipement affectent consid érablement la précision dimensionnelle des pièces [96]. Pendant ce temps, les propri ét és des mat ériaux d'encre et les param ètres de processus sont des entr ées de la mod élisation de processus DIW. Ainsi, ce chapitre présente les recherches sur la caract érisation des propri ét és des mat ériaux d'encre et la s élection des param ètres de processus pour fournir la base des entr ées de mod élisation.

Pour la caractérisation des propriétés du matériau de l'encre, la densité, la tension superficielle, l'angle de contact statique et les propriétés rhéologiques sont obtenues pour l'encre utilisée.

Pour la s dection des param dres de processus. R écemment, la s dection des param dres de processus DIW a étémen ée par de nombreux chercheurs [98, 158, 159]. Cependant, toutes ces études ont simplement d étermin é une fen être d'imprimabilit é au lieu d'une valeur optimale et peu d'études sont disponibles pour l'analyse de l'importance des param dres de processus et l'optimisation pour DIW. Par cons équent, il est important d'étudier l'impact de chaque param dre de processus et de trouver le réglage optimal des param dres de processus pour am éliorer la précision dimensionnelle des pi des fabriqu ée en DIW.

La méhode Taguchi [123] et les méhodes d'apprentissage automatique (ML) [108, 160] ont ét élargement utilis és pour contr ĉier les param ètres de processus de l'impression 3D bas ée sur l'extrusion de matériaux. Les méhodes ML permettent la sélection appropriée des param ètres avec peu d'analyses de processus, mais nécessitent un grand ensemble de donn ées, du temps et des ressources informatiques suppl émentaires [133]. La technique de Taguchi est plus efficace [161] avec une réduction significative du temps et du coût expérimentaux [126] et elle peut déterminer la signification de chaque param ètre par analyse de variance (ANOVA) [162]. Pour effectuer l'optimisation des param ètres du processus DIW avec un minimum de matériel et de temps, la méhode Taguchi est adopt ée dans cette th èse.

Les propri é és des mat ériaux d'encre sont caract éris és pour l'encre utilis ée dans cette th èse. Ensuite, les param ètres de processus sont s dectionn és pour l'encre utilis ée dans l'imprimante 3D DIW. En particulier, dans la s dection des param ètres de processus, nous identifions les param ètres de processus DIW par des analyses d'impression et proposons une m éthode d'optimisation en deux étapes pour optimiser les param ètres de processus DIW pour la pr écision dimensionnelle des couches imprim ées et analyser l'importance de chaque param ètre de processus (Figure 3.5). Pour v érifier la m éthode, des tests de confirmation sont effectu és en tenant compte de la comparaison des conditions et de la robustesse de la méhode sur d'autres formes. Ainsi,ces tests comparent l'adaptabilit é des param ètres dans l'impression de pi èces 3D à partir des analyses des couches imprim és pour la méhode propos é et de l'adaptabilit é des param ètres dans les constructions 3D fabriqu és à 100 % de remplissage ou avec porosit és.



Figure 3.5 Cadre de la m éhode en deux étapes propos ét pour optimiser les param ètres du processus DIW pour les couches imprim éts

# 4 Modélisation numérique, vérification expérimentale et analyse de processus DIW

Les r sultats de la mod disation pour DIW incluent le filament extrud é de forme libre (FEF), le filament d épos é (DF), le coin d épos é, la couche imprim ée et la pi èce 3D. Cette th èse porte sur les simulations num ériques des d éments les plus basiques en DIW : FEF, DF et coin d épos é

Premi à rement, la méhode du volume de fluide (VOF) est s dectionn é comme méhode de simulation numérique et elle est bri àvement décrite. Ensuite, des simulations numériques, des vérifications expérimentales et des analyses de processus DIW sont menées.

Pour la simulation num érique de FEF, il existe peu de travaux sur la mod disation et l'évaluation de FEF bas és sur des méthodes de simulation num érique pour DIW. La mod disation par simulation num érique du FEF doit tenir pleinement compte des propri ét és de l'encre et des param ètres de processus, car la qualit é du FEF d épend à la fois des propri ét és du mat ériau de l'encre et du r églage des param ètres de processus [119]. L'évaluation du FEF doit tenir compte à la fois du diam ètre moyen et de la stabilit écar ces deux indicateurs ont l'influence la plus significative sur la qualit é d'impression [172]. L'objectif de la mod disation de processus et de l'analyse de FEF bas és sur des simulations num ériques est d'éablir un mod è de FEF avec une méthode de simulation num érique, puis d'évaluer le FEF sur la base de ce mod è. Tout d'abord, un mod è de FEF est établi à l'aide d'une méthode de simulation num érique et deux indicateurs d'évaluation, le diam ètre moyen et la stabilit é sont propos és pour évaluer le FEF. Enfin, l'encre s dectionn é, Nivea Crème, est utilis és sous trois niveaux de vitesse de piston pour v érifier la simulation num érique. Apr ès v érification exp érimentale, le mod è et les indicateurs d'évaluation sont utilis és pour analyser l'effet de la vitesse du piston sur le FEF et trouver des fen êtres imprimables appropri és pour les param ètres de processus.

Pour la simulation num érique de DF, plusieurs chercheurs ont établi des mod des de prédiction num érique pour DF dans MEAM. Comminal et al. [147] ont établi un mod de num érique des filaments d'épos és dans le MEAM (Material Extrusion Additive Manufacturing) mais ce travail manquait de validation exp érimentale. Serdeczny et al. [173] ont utilis é une proc édure exp érimentale pour valider le mod de num érique et ont étudi é l'influence des conditions de traitement sur la section d'un fil imprim é par extrusion de mat ériau FA à travers un mod de num érique. Gohl et al. [144] ont utilis é un outil de simulation de dynamique des fluides computationnelle (CFD) pour étudier l'effet des param àres d'impression sur les filaments d'épos és en bio-impression. Goset et al. [174] ont présent é une étude num érique du

d ép ĉt d'un simple brin d'acide polylactique (PLA) par MEAM via un mod de CFD. Bien que les travaux pr & élents aient montr éque le DF est significativement influenc épar les param ères du processus, ils n'ont souvent pas r éussi àr éaliser des caract érisations quantitatives complètes de l'influence d étaill ét des param ètres du processus sur l'état de d ép  $\hat{\alpha}$  et la dimension du profil des filaments d'épos és. Pendant ce temps, il existe peu de travaux sur la prédiction num érique des filaments dépos és dans DIW en tenant pleinement compte des propri ét és du mat ériau de l'encre et du r églage des param ètres de processus. Ainsi, il est crucial et souhaitable d'étudier et de prédire pleinement l'état de dépôt et la dimension du profil des filaments déposés dans les processus DIW bas és sur la prédiction num érique. Dans ce chapitre, un mod de de prédiction num érique 3D am élior édes filaments d'épos és dans DIW est établi avec la méhode du volume de fluide (VOF) pour prédire l'état du dépôt et la dimension du profil des filaments déposés. Des exp ériences de d ép ât de filaments sont men és en utilisant l'encre s dectionn és pour v érifier le mod de propos é. En utilisant le mod de num érique propos é, l'état du d ép êt est divis é en trois états et la dimension du profil sous chaque état est prédite. L'effet des paramètres de processus, y compris la vitesse de la buse sans dimension et la hauteur sans dimension sur l'état du dép  $\hat{\alpha}$ et la dimension du profil, a ét équantifi épour la premi ère fois àl'aide de simulations num ériques. La simulation num érique du DF d émontre une approche efficace et économe en mat ériaux pour la prédiction de l'état de dépôt et de la dimension du profil du DF et l'étude des effets des param ètres de processus dans DIW avec des simulations num ériques informatis és.

Quand àla simulation num érique du coin d épos é pour bien comprendre le processus DIW et am diorer la qualit é g éom étrique des pi àces en DIW, les m éthodes de simulation num érique ont ét élargement utilis éts pour mod diser le processus MEAM [144, 147, 149, 175]. Gr âce aux avantages des simulations num ériques propos éts, les chercheurs ont évalu é avec succ às l'imprimabilit é de nouvelles encres pr épar éts, trouv é les param ètres de processus optimis és, analys é le processus d'extrusion de mat ériau et r éalis é le jumeau num érique du processus MEAM avec une faible consommation de mat ériau et de temps exp érimental [176- 178]. Comminal et al. ont simul éle d ép êt de brins [147] et le d ép êt de mat ériau le long d'un parcours d'outil avec un coin pointu [149] avec des mod èles de dynamique des fluides computationnelle (CFD) pour étudier l'effet des param ètres de processus sur les filaments et les coins d épos és, respectivement. Gohl et al. [144] ont men é des simulations informatiques pour DIW afin d'évaluer les encres nouvellement d évelopp éts. Tu et al. [175] ont établi un mod ète de filaments extrud és de forme libre avec simulation num érique, puis ils ont évalu éles filaments sur la base du mod èt pour DIW. Cependant, les travaux ant érieurs [149] pour la simulation num érique des coins d épos és ne pouvaient r éaliser la simulation de coin que sous la condition d'un petit angle inf érieur à 90 ° mais n'ont pas r éussi à r éaliser la simulation de coin de n'importe quel angle. Ainsi, pour surmonter les limites des recherches pr éc édentes sur la simulation num érique des coins d épos és et r éaliser pleinement la mod élisation du processus DIW bas ée sur l'application de la simulation num érique, il est crucial et n écessaire de proposer une simulation num érique am élior ée pour mod éliser les coins d épos és de n'importe quel angle. Dans ce chapitre, des simulations num ériques 3D de coins d épos és de n'importe quel angle dans DIW sont établies avec la m éthode VOF et des exp ériences de d ép ét de coin sont men ées à l'aide de l'encre s électionn ée pour valider la simulation num érique propos ée. La simulation num érique du coin de d ép ét surmonte la limitation des travaux de recherche ant érieurs dans la simulation num érique des coins d épos és et d émontre une approche efficace pour la pr édiction des coins d épos és de n'importe quel angle dans DIW

Dans ce chapitre, des simulations num ériques des él éments les plus él émentaires de DIW, y compris FEF (Figure 4.2), DF (Figure 4.7) et le coin d épos é (Figure 4.16), sont d évelopp és et des v érifications exp érimentales sont effectu és pour v érifier les simulations num ériques propos és (Figure 4.4 and Figure 4.9). Sur la base des simulations num ériques propos és, des analyses de processus de DIW sont men és.



Figure 4.2 Mod de g éom érique de FEF en simulation num érique pour DIW : (a) dimensions du mod de g éom érique ; (b) mod de 3D établi au moment initial ; (c) mod de axisym érique 2D simplifi étau temps initial



Figure 4.7 Mod disation num érique du profil 3D du DF : (a) mod de g éom érique 3D ; (b) les param dres critiques du mod de ; (c) maillages g én ér és ; (d) condition initiale de la fraction de phase



Figure 4.16 Mod disation num érique du profil 3D des coins d épos és : (a) mod de g éom érique 3D ; (b) maillages g én ér és ; (c) condition de vitesse dans les substrats ; (d) condition initiale de la fraction de phase



Figure 4.4 Configuration de validation exp érimentale pour la simulation num érique de FEF : (a) production de FEF à l'aide d'une imprimante 3D DIW et observation de FEF à l'aide d'une cam éra ; (b) outil d'extrusion dans l'imprimante DIW 3D



Figure 4.9 Montage exp érimental pour des exp ériences de d épôt de filaments et des exp ériences de d épôt de coins

Pour la simulation num érique de FEF, un mod de num érique de FEF est établi avec une méhode de simulation num érique, puis le FEF est évalu é sur la base de ce mod de. Deux indicateurs d'évaluation, diam dre moyen et stabilit é, sont propos és pour évaluer le FEF. L'encre s dectionn ée Nivea Cr ème est utilis ée pour v érifier la méhode. Le mod de num érique établi de FEF est v érifi é car la forme dans la simulation est conforme aux r ésultats exp érimentaux et la précision de la prédiction du diamètre est meilleure que 0,08 mm. Après v érification exp érimentale, le mod de et les indicateurs d'évaluation sont utilis és pour traiter les deux questions de l'analyse de processus pour FEF dans DIW comme suit :

(1) Analyser l'effet de la vitesse du piston sur le FEF : il existe une vitesse minimale du piston, 2 mm/s pour Nivea Cr ème pour le r églage de ve, pour produire un FEF continu et stable ; les diam ètres moyens de FEF diminuent avec l'augmentation de la vitesse du piston. La stabilit é diminue d'abord puis augmente avec la vitesse du piston augmente ;

(2) Trouvez des fen êtres imprimables appropri éts pour les param ètres de processus : la fen être imprimable de r églage de ve est de 5 mm/s à 15 mm/s pour Nivea Cr ème.

Pour la simulation num érique de DF, l'influence d étaill ét des param ètres de processus sur l'éat de d'épôt et la dimension du profil n'a pas été entièrement caractérisée quantitativement dans les précédents travaux de prédiction numérique pour le DF de DIW. Dans ce chapitre, l'effet des param ètres de processus sur l'état du dép êt et la dimension du profil a été quantifié sur la base d'une prédiction num érique. Un mod de num érique 3D am élior éest établi en utilisant la méthode VOF et en considérant les propriétés globales du matériau d'encre. Le modèle num érique 3D am élior é surmonte le problème des modèles 2D simplifiés précédents dans la prédiction de la section transversale. Il surmonte également la lacune des mod des num ériques 3D pr & édents en ignorant les propri ét és importantes du mat ériau telles que le coefficient de tension superficielle et l'angle de contact statique qui limitent la précision de la prédiction. Les param ètres de processus critiques sont identifi és comme étant la vitesse sans dimension de la buse (V\*) et la hauteur sans dimension (H\*). Sur la base de la prédiction num érique, l'état de dépôt est caractérisé en trois types nommés sur-dépôt, dépôt pressé et dépôt de forme libre (Figure 2.9) et la dimension du profil sous chaque état de dépôt est prédite. L'efficacité de la prédiction num érique pour les filaments d'épos és est valid ée car ses r ésultats sont coh érents avec les r sultats exp érimentaux et ils sont également coh érents avec les r sultats id éaux (th éoriques). La précision de la prédiction num érique pour la dimension du profil est v érifi éc car les erreurs relatives maximales de largeur et de hauteur entre les r sultats exp érimentaux et simul s sont respectivement de 10,13 % et 7,37 %, ce qui est significativement am dior é par rapport aux

valeurs rapport ées de 20 % et 28 % dans la litt érature. L'erreur relative maximale de la prédiction num érique pour la dimension du profil appara î au bord de la fen être imprimable.

Sur la base de la prédiction num érique, les effets des param ètres de processus DF sont également étudi és. L'état de d ép  $\hat{\alpha}$  commence du sur-d ép  $\hat{\alpha}$  au d ép  $\hat{\alpha}$  press é et enfin au d ép  $\hat{\alpha}$  de forme libre (Figure 2.9) lorsque V\* et H\* augmentent alors que la vitesse moyenne de l'encre dans la buse n'a pas d'effet significatif sur l'éat de dépôt et la dimension du profil. L'éat de d ép ôt doit être pris en consid étation pour l'effet des param ètres de proc éd é sur la dimension du profil : la largeur diminue avec V\* en d  $\phi \hat{\alpha}$  sous pression et en d  $\phi \hat{\alpha}$  de forme libre ; la hauteur reste la même avec V\* en d  $\notin \hat{\alpha}$  press é alors qu'elle diminue avec V\* en d  $\notin \hat{\alpha}$  de forme libre ; la largeur diminue avec H\* en d $\phi \hat{\alpha}$  sous pression tandis qu'elle reste la même avec H\* en d  $\phi$   $\hat{\alpha}$  de forme libre ; la hauteur augmente avec H\* en d  $\phi$   $\hat{\alpha}$  press é alors qu'elle reste la m  $\hat{\alpha}$ me avec H\* en d ép ĉt de forme libre. La simulation num érique et l'analyse de processus propos ées pour DF caract érisent l'état de d ép êt et étudient la dimension du profil dans chaque état de d ép êt sur la base de l'utilisation de la prédiction num érique. La simulation num érique de DF suggère une prédiction num érique efficace et économe en ressources pour l'état de d ép  $\hat{\alpha}$  et la dimension du profil du DF et l'éude des effets des paramètres de processus dans DIW. Elle fournit également une base viable pour les travaux futurs sur l'daboration de la mod disation num érique de l'ensemble du processus d'impression 3D DIW.

Pour la simulation num érique des coins d épos és, les travaux de recherche ant érieurs pour la simulation num érique des coins d épos és ne pouvaient r éaliser la simulation de coin que dans des conditions de petit angle et n'ont pas r éussi à r éaliser la simulation de coin de n'importe quel angle. Dans ce chapitre, une simulation num érique 3D am élior és des coins d épos és est établie en utilisant la m éhode VOF et en consid érant les propri ét és globales du mat ériau d'encre. La simulation num érique 3D am élior és surmonte la limitation des travaux pr és élents et r éalise une mod élisation de coin d épos é de n'importe quel angle en construisant deux zones de calcul (Figure 4.16) o ù deux vitesses de buse avec l'angle de coin sont appliqu és sur les substrats de deux zones de calcul. L'efficacit édu mod èle num érique propos éest valid ée par des exp ériences de d ép êt de coins en utilisant l'encre s électionn ée dans une imprimante DIW 3D car les angles de coin simul és correspondent bien aux angles exp érimentaux et la valeur maximale de MDDSEO est de 1,06  $\pm$ 0,06 mm. On observe que la pr écision de la simulation dans les coins est inf érieure àcelle dans les filaments. La raison de ce ph énom ène est due àla diff érence entre la vitesse de la buse appliqu ée sur le substrat dans la simulation num érique et la vitesse r étlle de la buse dans les exp ériences uniquement pour la r égion d'angle, car la buse a besoin d'un

processus de d éc d ération et d'acc d ération uniforme pour changer la direction de la vitesse de la buse dans la pratique. impression. Le MDDSEO des coins d épos és diminue à mesure que l'angle de coin augmente.

Les simulations num ériques de FEF, DF et des coins d'épos és suggièrent une simulation num érique efficace pour les sorties de mod disation dans DIW qui pourrait être utilis ée dans les travaux d'analyse de processus DIW, y compris l'évaluation de l'imprimabilit é de nouvelles encres pr épar ées, l'optimisation des param ètres de processus et l'établissement d'un jumeau num érique. Ils fournissent également une base viable pour les travaux futurs sur l'étaboration de la mod élisation num érique de l'ensemble du processus d'impression 3D DIW.

# 5 Conclusion et perspectives

## 5.1 Conclusion

La compr hension et l'analyse du processus DIW n'ont pas été entièrement étudiées, ce qui limite la précision de fabrication et la promotion de l'application de cette technique. La simulation numérique est l'un des outils les plus puissants d'analyse de processus en FA. L'analyse de processus bas ét sur des simulations numériques présente des avantages en termes d'économie de temps de matériau/d'essai et de capture facile de la valeur des paramètres de processus critiques qui sont difficiles à obtenir par des mesures expérimentales. La recherche sur la modélisation des processus et l'analyse de DIW bas ét sur des simulations numériques fournira un soutien important pour le développement et l'orientation de DIW. Cependant, il existe actuellement peu de travaux systématiques sur la modélisation et l'analyse des processus bas ét sur des simulations numériques pour DIW. Pour combler cette lacune, cette thèse effectue des recherches sur la modélisation et l'analyse des processus DIW .

Dans le chapitre 2, l'examen syst énatique de la litt érature sur le DIW est effectu éd'abord pour r ésumer les caract éristiques, le d éveloppement, les d éfis et les solutions aux d éfis de DIW et un problème insuffisamment r ésolu - la difficult é de trouver rapidement des paramètres de processus appropri és pour l'encre pr épar ée - est d étermin é comme la question de recherche de cette thèse. Pour r ésoudre la question de recherche, la piste de la mod élisation et l'analyse des processus DIW est poursuivie pour r ésoudre le problème. Ensuite, une revue de litt érature sur la mod élisation et l'analyse de processus DIW est r éalis ée. Les entrées et les sorties de la mod élisation des processus sont r ésumées et les méthodes de mod élisation num érique des processus sont s électionn ées comme les plus appropri ées pour la mod élisation des processus et l'analyse de DIW. Cependant, il existe actuellement peu de travaux syst ématiques sur la mod disation et l'analyse des processus bas és sur des simulations num ériques pour DIW. Sur la base de l'examen, l'objectif de cette thèse est formul écomme suit : contribuer à la mod disation et à l'analyse de processus DIW sur la base de simulation num érique.

Dans le chapitre 3, l'encre Nivea Cr àme et une imprimante 3D DIW àpiston sont choisies pour v érifier les simulations num ériques propos ées. Avant la simulation num érique, les propri ét és des mat ériaux d'encre sont caract éris ées et le r églage optimal des param àtres de processus est calcul é pour fournir la base des entr ées de mod élisation. Pour la caract érisation des propri ét és du mat ériau de l'encre, la densit é, la tension superficielle, l'angle de contact statique et les propri ét és rh éologiques sont obtenues pour l'encre utilis é. Pour la s élection des param àtres de processus, les param àtres de processus DIW sont identifi és par des analyses de processus et une m éthode en deux étapes est propos ée pour optimiser les param àtres de processus. Diw pour la précision dimensionnelle et analyser l'importance de chaque param àtres de processus. Des v érifications exp érimentales v érifient la m éthode de s élection des param àtres de proc ét é propos ée et la robustesse de celle-cisur d'autres formes et d'autres mat ériaux. Il a été également analysél'adaptabilit é des param àtres dans l'impression de pi àces 3D à partir des analyses des couches imprim és selon la m éthode propos ée et l'adaptabilit é des param àtres dans les constructions fabriqu és à 100 % de remplissage ou avec des porosit és.

Dans le chapitre 4, des simulations num ériques des param ètres principaux de DIW, y compris FEF, DF et le coin d'épos é, sont propos ées et des v érifications exp érimentales sont men ées pour v érifier les simulations num ériques propos ées. Sur la base des simulations num ériques propos ées, des analyses de processus DIW sont men ées.

Pour la simulation num érique de FEF, le mod de num érique établi de FEF est v érifi é car la forme dans la simulation est conforme aux r ésultats exp érimentaux et la pr écision de pr édiction du diam dre est inf érieur à0,08 mm. L'analyse du processus bas ée sur la simulation num érique du FEF montre que : 1) il existe une vitesse de piston minimale, 2 mm/s pour Nivea Cr ème pour produire un FEF continu et stable ; 2) les diam dres moyens de FEF diminuent avec l'augmentation de la vitesse du piston et la stabilit é diminue d'abord puis augmente quand la vitesse du piston augmente ; 3) des fen dres imprimables appropri ées sont trouv ées dans l'intervalle de 5 mm/s à15 mm/s pour Nivea Cr ème.

Pour la simulation num érique de DF, l'effet des param ètres de processus sur l' état de d ép ôt et la dimension du profil a ét équantifi ésur la base de la prédiction num érique de DF. Un mod ète num érique 3D am élior é est établi en utilisant la m éthode VOF et en consid érant les propri ét és globales du mat ériau d'encre. Le mod ète num érique 3D am élior é surmonte le probl ème des mod des 2D simplifiés précédents dans la prédiction de la section transversale. Il surmonte aussila lacune des mod des num ériques 3D précédents qui ignorent les propriétés importantes du matériau telles que le coefficient de tension superficielle et l'angle de contact statique qui limitent la précision de la prédiction. Les paramètres de processus critiques sont identifiés comme étant la vitesse sans dimension de la buse et la hauteur sans dimension. Sur la base de la prédiction numérique, l'état de dépôt est caractériséen trois types nommés sur-dépôt, dépôt presséet dépôt de forme libre et la dimension du profil sous chaque état de dépôt est prédite.

Pour la simulation num érique des coins d épos és, les travaux de recherche ant érieurs pour la simulation num érique des coins d épos és ne pouvaient r éaliser la simulation de coin que dans des conditions de petit angle et n'ont pas r éussi àr éaliser la simulation de coin de n'importe quel angle. Une simulation num érique 3D am élior ée des coins d épos és est établie en utilisant la m éhode VOF et en consid érant les propri étés globales du mat ériau d'encre. La simulation num érique 3D am élior ée surmonte la limitation des travaux précédents et réalise une mod élisation de coin d épos é de n'importe quel angle en construisant deux zones de calcul o ù deux vitesses de buse avec l'angle de coin sont appliqu ées sur les substrats de deux zones de calcul. L'efficacit é du mod éle num érique propos é est valid ée par des exp ériences de d ép ét de coins en utilisant l'encre s électionn ée dans une imprimante DIW 3D car les angles de coin simul és correspondent bien aux angles exp érientaux et la valeur maximale de MDDSEO (deviation between simulated and experimental outlines) est de 1,06  $\pm$  0,06 mm. On observe que la précision de simulation dans les coins est inférieure à celle dans les filaments et le MDDSEO des coins d épos és diminue quand l'angle de coin augmente.

En conclusion, cette thèse mène de la recherche à travers des revues systématiques de la litt érature et elle propose un cadre outill épour la caract érisation des propri étés des matériaux d'encre, la sélection des paramètres du processus, les simulations numériques, la vérification expérimentale et l'analyse des processus DIW. Cette thèse propose une simulation numérique efficace pour les sorties de modélisation dans DIW qui pourrait être utilisée dans les travaux d'analyse de processus DIW, y compris l'évaluation de l'imprimabilité de nouvelles encres préparées, l'optimisation des paramètres de processus et l'établissement d'un jumeau numérique, ce qui est utile pour la compréhension du processus et l'analyse de processus DIW.

#### 5.2 **Perspectives**

A la suite des travaux pr ésent és au chapitre 1-4, bien d'autres perspectives peuvent être envisag és. Parmi ceux que j'esp ère suivre, il y a :

Pour la s dection des param àres de processus, l'analyse quantitative des objets imprim és est limit ée et la thèse n'obtient pas de relation quantitative entre l'entr ée et la sortie bas ée sur la méhode expérimentale. Les travaux futurs mèneront une évaluation quantitative des objets imprim és à l'aide de la méhode de vision par ordinateur et une relation quantitative entre l'entr ée et la sortie sera propos ée sur la base des donn ées quantitatives à l'aide de la méhodologie de surface de réponse.

Pour les simulations num ériques de DIW, la thèse n'établit pas de simulations num ériques de couches imprim ées et de pièces 3D. Les travaux futurs établiront des simulations num ériques des couches imprim ées et des pièces 3D pour r'éaliser la mod élisation de toutes les sorties pour DIW, y compris FEF, DF, coins d'épos és, couches imprim ées et pièces 3D.

Pour l'analyse du processus de DIW, la thèse n'analyse pas complètement le processus dans l'évaluation de l'imprimabilité des nouvelles encres préparées, l'optimisation des paramètres du processus et la mise en place du jumeau numérique. Les travaux futurs mèneront un travail complet d'analyse des processus, y compris l'évaluation de l'imprimabilité des nouvelles encres préparées, l'optimisation des paramètres du processus et l'établissement d'un jumeau numérique, ce qui est utile pour la comprénension et l'analyse du processus DIW.

# Listes de publications

# Articles de journaux :

[1] **Yongqiang Tu**, Javier A. Arrieta-Escobar, Alaa Hassan, et al. Optimizing Process Parameters of Direct Ink Writing for Dimensional Accuracy of Printed Layers [J]. 3D Printing and Additive Manufacturing, 2021, published online. DOI: 10.1089/3dp.2021.0208

 [2] Yongqiang Tu, Alaa Hassan, Javier A. Arrieta-Escobar, et al. Modeling and evaluation of freeform extruded filament based on numerical simulation method for direct ink writing [J]. The International Journal of Advanced Manufacturing Technology, 2022, 120: 3821-3829. DOI: 10.1007/s00170-022-08999-3

[3] **Yongqiang Tu**, Alaa Hassan, Ali Siadat, et al. Numerical simulation and experimental validation of deposited corners of any angle in direct ink writing [J]. The International Journal of Advanced Manufacturing Technology, 2022, 123: 559-570. DOI: 10.1007/s00170-022-10195-2

[4] **Yongqiang Tu**, Alaa Hassan, Ali Siadat, et al. Analytical modeling of deposited filaments for high viscosity material-based piston-driven direct ink writing [J]. The International Journal of Advanced Manufacturing Technology, 2022, 123: 3387-3398. DOI: 10.1007/s00170-022-

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# Articles de conférence:

[1] **Yongqiang Tu**, Javier A. Arrieta-Escobar, Alaa Hassan, et al. Predictive modeling of extruded filament in the air for bioink in direct ink writing using numerical simulation [C]. Procedia CIRP, 2022, 112(4): 394-399. DOI: 10.1016/j.procir.2022.09.026

[2] **Yongqiang Tu**, Alaa Hassan, Ali Siaddat, et al. Multi-objective optimization based viscosity prediction for inks in direct ink writing numerical simulations [C]. Intelligent Networked Things, CINT 2022, Communications in Computer and Information Science, 2022, 1714: 147-157. DOI: 10.1007/978-981-19-8915-5\_13

[3] **Yongqiang Tu**, Huiyun Gong, Alaa Hassan, et al. Computer vision-based evaluation of dimensional accuracy for MEAM in new product development [C]. Accepted. // The CIRP Design conference, 2023, Sydeny, NSW, Australia.

**English Version** 

# **Chapter 1: General Introduction**

# 1.1 Context and objective of the present study

Additive manufacturing (AM) is an advanced manufacturing technology that directly prints three-dimensional (3D) parts by stacking material layer by layer based on a digital 3D computer-aided design (CAD) model [1-5]. Compared with the traditional manufacturing techniques such as forging, casting, welding and machining (turning, milling, planing, grinding, etc.), AM has the advantages of digitization, material saving, material diversification and the ability to easily manufacture complex parts, which meet the requirements of high precision, structural freedom and customizability for the development of new materials and new structures in tissue engineering, medicine, rubber engineering, ceramic engineering, sensors, aviation, aerospace, electronics, food and other industrial applications [6-10]. According to ISO/ASTM 52900 (2015), AM is divided to seven categories based on the working principle: binder jetting (BJ), directed energy deposition (DED), material extrusion (ME), material jetting (MJ), powder bed fusion (PBF), sheet lamination (SHL) and vat photo polymerization (VPP).

Direct ink writing (DIW) belongs to the material extrusion AM (MEAM) according to the working principle. The working principle of DIW is: first, the material is prepared in paste or slurry type with good printability named ink; then the ink is extruded from a nozzle into continuous filaments using mechanical force (piston or screw drive) or pneumatic force; and finally the filaments are deposited into layer-wise 3D parts [11]. Compared with other AM techniques, DIW has the outstanding advantages in diversity in materials and flexibility in equipment [12-14]. Due to the advantages, DIW has become one of the most popular AM techniques in recent years.

However, the process understanding and analysis of DIW have not been fully studied, which limits the manufacturing accuracy and application promotion of this technique. Both ink material properties and process parameters setting influence the printed results of DIW. Ink material properties include density, surface tension efficient and rheological properties. Process parameters include nozzle inner diameter, syringe diameter, piston speed, nozzle speed and layer height. Thus, it is a challenge to establish a complete and accurate model for DIW due to the complex relationship between inputs and outputs for DIW. In recent studies, due to the lack

of process understanding and analysis of DIW, scholars need to go through numerous trials to find a printable window of ink properties and process parameters suitable for DIW to obtain the printing quality that meets the requirements of use [15-17]. This largely increases cost and reduces application attractiveness of DIW. To solve this problem, it is of critical to do research on process modelling and analysis for DIW to fully understand this process and improve the usability of DIW. In conclusion, the research question in the application of DIW: it is of critical to establish a complete and accurate model for DIW because the process understanding and analysis of DIW have not been fully studied, which limits the manufacturing accuracy and application promotion of this technique; however, it is difficult to establish the model of DIW due to the complex relationship between inputs and outputs for DIW.

Numerical simulation is one of the most powerful tools in process analysis in AM. Process analysis based on numerical simulations has advantages in saving material/trial time and easily capturing critical process parameters value which are difficult obtained by experimental measurements. The research on process modeling and analysis of DIW based on numerical simulations will provide important support for the development and guidance of DIW. However, there is currently few systematic research works on process modeling and analysis based on numerical simulations for DIW. To bridge this gap, the objective of this thesis is to improve process modeling and analysis for DIW based on numerical simulations.

## **1.2 Research contents**

Specially, DIW process is influenced by both ink material properties and process parameters. Besides, ink material properties and process parameters are input conditions in numerical simulations. Thus, firstly, ink material properties characterization and process parameters selections are studied and the research results are used as input conditions for the numerical simulations. Then, numerical simulations for DIW are conducted. As one of the AM technologies, as shown in Figure 1.1, the whole process steps of DIW include:

- Step 1: 3D geometrical modeling using top-down design in 3D modeling software like Solidworks, ProE, UG, CATIA, 3DMAx, etc.; or using reversal design based on the 3D model data from virtual reality technology or 3D scanner;
- Step 2: G-code generation by importing STL format of 3D geometrical model and setting process parameters in Slicer software;
- Step 3: Printing in a DIW 3D printer using the generated G-code through the layerwise manufacturing process.

Specially, DIW can print arbitrarily complex 3D parts through ink extrusion, points-to-line, lines-to-layer, and layers-to-3D part processes as illustrated in Step 3 chart in Figure 1.1. Among this process, freeform extruded filament (FEF), deposited filament (DF) and deposited corner are the most basic and critical elements (Step 3 chart in Figure 1.1). Thus, the thesis focuses on the numerical simulations and process analyses of these basic and critical elements: FEF, DF and deposited corner.

In conclusion, to achieve the objective of the thesis, research contents include:

- Research on ink material properties characterization and process parameters selection;
- Research on numerical simulation of basic and critical elements in DIW including FEF, DF and deposited corner;
- Experimental verifications of the proposed numerical simulations;
- Process analysis based on the proposed numerical simulations.



Figure 1.1 Process illustration of DIW and summarized research object in this thesis: (a)
CAD model built in 3D modeling software; (b) CAD model from 3D scanner; (c) CAD model saved as STL format; (d) 3D model imported in Slicer software; (e) process parameters setting in Slicer software; (f) generated G-code using Slicer software; (g) mechanical composition of DIW 3D printer; (h) ink in the syringe; (i) real photo of DIW 3D printer; (j) ink extrusion process; (k) points-to-line process; (l) lines-to-layer process; (m) layers-to-3D part process; (n) basic and critical elements in DIW process; (o) summarized research object

## **1.3 Thesis structure**

This thesis is structured in five chapters and the content of each chapter is briefly introduced as follows:

Chapter 1 gives an overview of the research context and objective. Based on the research objective, research contents are summarized. Finally, the thesis structure is outlined.

Chapter 2 studies the state of the art, a systematic literature review of DIW is conducted firstly to summarize features, development, challenges and solutions for challenges of DIW.As results, insufficiently solved problem is determined and the related research question of this thesis is formalized. To answer the research question, process modeling and analysis for DIW is selected as approach. Afterwards, a literature review of process modeling and analysis for DIW is conducted. Inputs and outputs of process modeling of DIW are summarized and numerical process modeling methods are selected as the most suitable method for process modelling and analysis of DIW. Finally, the objective of this thesis is determined based on the literature review.

Chapter 3 presents the works on ink material properties characterization and process parameters selection to provide the basis for modeling inputs. For ink material properties characterization, density, surface tension, static contact angle and rheology properties are obtained for the used ink. For process parameters selection, DIW process parameters are identified through printing analyses and a two-step optimization method is proposed to optimize DIW process parameters for dimensional accuracy of printed layers and analyze the significance of each process parameter.

Chapter 4 presents the numerical simulations of FEF, DF and deposited corners in DIW. Firstly, the numerical simulation method, volume of fluid (VOF), is introduced. Then, numerical simulations of FEF, DF and deposited corners are presented through geometrical modeling, meshes generation, and boundary conditions determination. Then, experimental verifications are conducted to verify the proposed numerical simulations. Finally, process analysis is conducted based on the proposed numerical simulation model.

Chapter 5 presents the conclusion and perspectives of the thesis.

# **Chapter 2:** State of the art

# **2.1 Introduction**

In recent years, DIW has attracted great attention both from academia and industry, and DIW has become one of the most popular AM techniques. However, as a technique that has developed rapidly in recent years, there are still many problems needed to be solved in the practical use of DIW and a thorough state-of-art of DIW is critical to understand its development status and problem. Based on the summarized problem in the state-of-art of DIW, process modeling and analysis using numerical simulations is selected as an effective way to solve the insufficiently solved problem. Thus, a literature review on process modeling and analysis using numerical simulations for DIW is further carried out and research gaps are summarized based on the literature review. Based on the summarized research gaps, detailed objectives are proposed.

The rest of this chapter is organized as follows. Section 2.2 presents the systematic literature review of DIW. The review introduces the criticality of AM technology in Section 2.2.1 firstly. Then, the most commonly used AM techniques are introduced and features of each AM technique are summarized to analyze the advantages and suitable applications of DIW in Section 2.2.2. Afterward, development, challenges and solutions for challenges of DIW are reviewed and an insufficiently solved problem is determined as the research question of this thesis in Section 2.2.3. To solve the research question, process modeling and analysis for DIW is selected as approach. Thus, process modeling and analysis for DIW is reviewed in Section 2.3.1 inputs and outputs of process modeling are summarized in Section 2.3.1 and process modeling methods are reviewed in Section 2.3.2. Based on the research gaps summarized in the literature review, Section 2.3.3 identifies the objective of this thesis.

# 2.2 A literature review on DIW

# 2.2.1 Criticality of AM technology

Thanks to the layer-wise manufacturing principle, AM is able to build materials into freeform and complex geometries from digitally modeled geometrical objects directly without requiring additional tooling [18] to realize complex structural and functional requirement of

parts. Meanwhile, AM can largely reduce cost of manufacturing by reducing material consumption and labor cost based on automated direct printing. Therefore, AM technology has gained great attention over the past five years in applications ranging from the industrial equipment, to aerospace, automobile making, consumer electronics, biomedicine, education & research, military use, building and other uses [19-23] (Figure 2.1 (a)).Over the past several years, the AM production cost has gone down in terms of low-cost step motors, mechanical components as well as equipment, such as lasers, digital projectors, precision extruders, and a growing library of printable materials has been established for feed stocks. AM's significant business potential and applications. AM industry has now experienced significant growth and production of additively manufactured parts has been increasing at an average annual rate of about 26% for the past 10 years (Figure 2.1 (b)) [24].



Figure 2.1 (a) AM applications and production share in various sectors and (b) Annual production of AM parts from independent service providers worldwide (in million US dollars)[24]

# 2.2.2 AM techniques

The AM techniques are divided into seven categories based on the working principle according to ISO/ASTM 52900 (2015). As shown in Figure 2.2, the commonly used AM techniques include: binder jet 3D printing (BJ3DP), laminated object manufacturing (LOM), fused deposition modeling (FDM), direct ink writing (DIW), inkjet printing (IJP), selective laser sintering (SLS), selective laser melting (SLM), powder based directed energy deposition (PBDED), wire based directed energy deposition (WBDED), stereolithography (SL), digital light processing (DLP) and two-photon polymerization (TPP).

#### 2.2.2.1 Binder jet 3D printing (BJ3DP)

BJ3DP belongs to binder jetting AM and BJ3DP is a process in which a liquid binder is jetted on layers of powdered materials, selectively joined, and then followed by densification process [25]. As illustrated in Figure 2.2 (a), in this process, solid powder is spread on a powder bed and a printing head ejects a liquid binder that binds the powder together in the areas same as the slicer of the 3D part in a layer-by-layer sequence. The resolution of BJ3DP is determined by the size and shape of the powder material as well as the feature size of the binder droplet (the typical resolution of BJ3DP is few 100 µm to mm) [26, 27]. The binder solution should have appropriate rheological properties for smooth ejection through the print head. A typical feature generated by the process is a high residual porosity in the printed part, due to the requirement of using rather coarse powders to enable the spreading of defect-free layers. Furthermore, thin features cannot be easily produced using this method [28]. BJ3DP provides very good flexibility in geometry design and is best for the printing of parts for which precision in resolution and surface finish is less of a requirement [29].

#### 2.2.2.2 Laminated object manufacturing (LOM)

LOM belongs to sheet lamination AM and LOM is a process in which layers of adhesivecoated paper, plastic, or metal laminates are successively glued together and cut to shape with a knife or laser cutter (Figure 2.2 (b)). Objects printed with this technique may be additionally modified by machining or drilling after printing. Finally, 3D parts can be obtained after binder removal and sintering. Typical layer resolution for this process is defined by the material feedstock and usually ranges in thickness from one to a few sheets of copy paper. The LOM technique may suffer poor surface quality, delamination, anisotropy along the build direction and planar direction due to weak interfacial bonding between the sheets [30]. The resolution of LOM is in mm. In terms of complexity, LOM is restricted to the fabrication of structures with simple geometries and relatively larger dimensions. Also, the removal of unprocessed material is time-consuming and expensive, causing substantial amount of material waste [31].



Figure 2.2 Classification and illustrations of different commonly used AM techniques: (a) BJ3DP, (b) LOM, (c) FDM, (d) DIW, (e) IJP, (f) SLS/SLM, (g) PBDED, (h) WBDED, (i) SL, (j) DLP, (k) TTP

#### 2.2.2.3 Material extrusion AM (MEAM)

MEAM has recently become widespread for the layer-by-layer fabrication of 3D parts and components even with highly complex shapes. This technology involves extrusion through a nozzle by means of a plunger-, filament- or screw-based mechanism. MEAM offers greater design freedom, larger building volumes and more cost-efficient production than liquid and powder-based AM processes [32]. This technology mainly contained two techniques: fused deposition modeling (FDM) and direct ink writing (DIW).

#### (1) Fused deposition modeling (FDM)

FDM process involves the extrusion of thermoplastic composite filaments melted by a moving nozzle which is heated with temperature kept above the glass transition temperature of the polymeric material involved onto a build platform in a layer-by-layer fashion, and the material solidifies immediately on the previously printed layer due to cooling to create 3D objects (Figure 2.2 (c)). The major difference compared with DIW is that heating is involved in the FDM process. The disadvantages of FDM are lower printing resolution (about 100  $\mu$ m), staircase effect and inherent anisotropy of the printed parts, mainly caused by the filament-based layer-by layer printing process [33].

#### (2) Direct ink writing (DIW)

As illustrated in Figure 2.2 (d), DIW is an extrusion-based method using a non-Newtonian viscous ink with composed rheological properties and configuration of liquid and solid phases as printing material at room temperature [9]. Similar to FDM, the resolution of DIW is also significantly influenced by the diameter of the nozzle, which can be in the range of dozens to hundreds of micrometers, leading to the staircase effect causing low resolution (100-1200  $\mu$ m for the x-y layer and 100-400  $\mu$ m for z resolution), poor surface finish and high anisotropy in geometrical and mechanical properties for the printed parts [34]. However, owing to the wide choice of material and low-cost process, DIW has become increasingly popular for the application needing high freedom in materials with relative low accuracy requirement.

#### 2.2.2.4 Inkjet printing (IJP)

IJP belongs to material jetting AM and this technique was originally introduced for office printing applications but have since then developed also into a valuable tool for research applications and for the fabrication of microstructures. As shown in Figure 2.2 (e), inkjet printing utilizes a dispensing unit to deposit small volumes of liquid material onto a substrate. The major advantage of this technology is the reliable handling of minute amounts of material which can be processed into defined droplets [35]. The resolution of IJP is around 50 μm. The

main limitation of IJP is the technique has limited capability of printing overhanging or hollow structures due to difficulty in support preparation [36, 37].

#### 2.2.2.5 Power bed fusion (PBF)

PBF AM uses either a laser or electron beam to melt and fuse material powder together, which main includes direct metal laser sintering (DMLS), electron beam melting (EBM), selective heat sintering (SHS), selective laser sintering (SLS) and selective laser melting (SLM). Among these techniques, SLS and SLM are most popular in PBF AM techniques as they have better quality in accuracy and mechanical properties.

#### (1) Selective laser sintering (SLS)

SLS belongs to PBF AM. SLS involves layer-by-layer spreading of powder, followed by selectively scanning and sintering using a high-power laser for bulk joining of the powder to build the final 3D part (Figure 2.2 (f)) [38]. After the SLS process is completed, the printed part is de-powdered and subjected to high temperature treatments for binder removal. SLS does not require extra support structure for hanging components, as the printed part is always embedded in the loose powder bed. The resolution of SLS is 20-150  $\mu$ m. SLS has been extensively used for the fabrication of a broad range of materials in powder form, such as polymers, metals and composite powders [39-41].

## (2) Selective laser melting (SLM)

SLM uses similar mechanism with a laser beam of much higher energy density to fully melt and fuse metallic powders to produce near net-shape parts with near full density (up to 99.9% relative density) in a single step (Figure 2.2 (f)) [42]. SLM is performed under controlled atmospheric conditions and has dominated the metal AM industry for its excellent quality in accuracy and mechanical properties, particularly for manufacturing median to large-size metallic components with topologically optimized structures [43-45]. The resolution of SLM is 20-100  $\mu$ m.

#### 2.2.2.6 Direct energy deposition (DED)

DED is a metal AM technology where an energy source – usually an electron beam, laser or arc – is directed toward a plate or other substrate material where it impinges with wire or powder feedstock material and melts, leaving deposited material on the substrate [46]. DED techniques are divided into two categories named powder based directed energy deposition (PBDED) (Figure 2.2 (g)) and wire based directed energy deposition (WBDED) (Figure 2.2 (h)) according to the feedstock in powder or wire [47, 48]. Both PBDED and WBDED contain a robotic arm and a source (electron beam, laser beam process or arc). DED can produce similar parts to those created with conventional machining. Thus, DED is commonly used in parts need to be for applications where conventional manufacture is expensive or slow with in the aerospace, defense, power and marine sectors [49, 50]. Moreover, DED is increasingly replacing conventional methods for the repair of parts such as the repair of damaged turbine blades or propellers [51].

#### 2.2.2.7 Vat photo polymerization (VPP)

VPP utilizes a localized energy source to fuse curable polymeric material for the layerwise fabrication of 3D geometry [52]. The most commonly used VPP techniques are stereolithography (SL), digital light processing (DLP) and two-photon polymerization (TPP). VPP has the highest resolution among AM techniques: both SL and DLP have resolution below 100 µm and TPP has resolution in sub µm.

#### (1) Stereolithography (SL)

SL has become vastly popular for its ability to produce high-accuracy, isotropic, and watertight prototypes and parts in a range of advanced materials with fine features and smooth surface finish [53]. As shown in Figure 2.2 (i), SL uses a vat of liquid photopolymers resin that can be cured [54]. The build plate moves in small increments and the liquid polymer is exposed to light where the Ultraviolet (UV) laser draws a cross-section layer by layer. The process repeats until a model is created. The object is 3D printed by pulling the object out of the resin (bottom-up) which creates space for the uncured liquid resin at the bottom of the container and can then form the next layer of the object.

#### (2) Digital light processing (DLP)

DLP is developed from SL [55]. The major difference of DLP from SLA is that DLP uses a projection of UV light or visible light from a digital projector to flash a single image of the layer across the entire resin at once [56, 57]. In DLP, the digital micro-mirror device (DMD) chip is one important component, which is composed of an array of reflective aluminium micro-mirrors that redirect incoming light from the UV source to project an image of a designed pattern or a layer of a 3D CAD model (Figure 2.2 (j)). The projection of an image that is composed of small square pixels called "voxels" passes through an optical lens and cures the photo-curable polymer resin.

#### (3) Two-photon polymerization (TPP)

TPP is a maskless direct laser writing technology [58]. In TPP, the light-matter interaction only takes place within the volume of a focused laser spot (Figure 2.2 (k)). The simultaneous

absorption of two photons in the focused spot triggers the locally confined polymerization of an exposed photoresist. The laser focus can be moved through the volume of the photoresist along all three spatial dimensions. Complex 3D structures are written along the laser's trajectory. Thanks to its versatility, TPP fabrication has applications in many fields, including micro optics, photonics, micromechanics, and biomedicine [59-61]. The advantage of TPP is that it has the highest resolution in AM techniques (sub µm). However, it has the disadvantage of slow speed and high cost.

#### 2.2.2.8 Features of each AM technique

Each AM technique has its own features, applicable materials, printing requirement and resolution. Various structural or functional parts manufacturing applications can find the most suitable AM technology according to the features and applicable materials of each AM technology. Features, applicable materials, feedstock form, forming method, printing requirement and resolution of each AM technique are summarized in Table 2.1[24].

AM technique	Features	Applicable materials	Feedstock form	Forming method	Printing requirements	Resolution
BJ3DP	Limited strength and rough surfaces	Metals, sand, ceramics	Slurry & Powder	Binder bonding	Dissolvable in solvents and act as binder	µm to mm
LOM	Low speed and large size, low precision, limited by binder	Paper, plastic, metals, ceramics	Sheets	Stacking and laser cutting	Sheets	mm
FDM	High speed and large size, low precision, limited by extrusion temperature	Thermoplastic polymers	Filament	Extrusion	In filament state	mm
DIW	High speed, low cost, wide choice of materials	Polymers, bio-ink, metals, cement, ceramics	Slurry	Extrusion	Appropriate viscosity and rheological properties	Few 100 µm to mm

 Table 2.1 Features, applicable materials, feedstock form, forming method, printing requirement and resolution of each AM technique [24]

AM technique	Features	Applicable materials	Feedstock form	Forming method	Printing requirements	Resolution
IJP	Less material quantity, limited by printable inks, low printing speed	Polymers, bio-ink, metals, ceramics	Slurry	Binder bonding	Low viscosity with rapid bonding	Few 100 μm to mm
SLS	Slow speed, high dimensional accuracy	Nylon, metals	Powder	Powder sintering	Meltable by laser	µm to mm
SLM	Slow speed, high dimensional accuracy	Metals	Powder	Powder fusion	Meltable by laser	µm to mm
PBDED	High speed, large size	Metals	Powder	Powder fusion	Meltable by source	µm to mm
WBDED	High speed, large size, low precision	Metals	Wire	Wire fusion	Meltable by source	mm
SL	Moderate speed, moderate cost, high efficiency, good surface quality	Resins, ceramics	Slurry	Linear polymerization	Dissolvable and UV photocurable moieties	Sub 100 µm
DLP	High speed, moderate cost, high efficiency, good surface quality	Resins, ceramics	Slurry	Linear polymerization	Dissolvable and UV photocurable moieties	Sub 100 µm
TPP	Slow speed, high cost, fine surface quality, highest printing precision	Resins, ceramics	Slurry	Non-linear polymerization	Dissolvable and two- photon absorption moieties	Sub µm

Table 2.1 (Continued) Features, applicable materials, feedstock form, forming method,printing requirement and resolution of each AM technique [24]

Comparisons of diversity in materials, cost, speed, resolution of each AM techniques are listed as follows:

(1) Diversity in materials

**DIW**> IJP >LOM>BJ3DP>FDM >SL, DLP, TPP>SLS>SLM, PBDED, WBDED (2) Cost SLM >SLS>PBDED >WBDED>TPP>SL>DLP>IJP>BJ3DP>LOM>FDM>DIW (3) Speed IJP, BJ3DP >DLP>LOM> DIW>FDM> WBDED>PBDED>SLM>SLS>SL>TPP (4) **Resolution** TPP>SL>DLP>SLM>SLS>PBDED>IJP>BJ3DP>DIW>FDM>WBDED>LOM (5) Manufacturing scales DIW, FDM, WBDED>IJP, BJ3DP>LOM>SLS, SLM, PBDED>SL, DLP>TPP (6) Ability to produce lightweight and optimized parts TPP>SL, DLP>SLM, SLS, PBDED>IJP>BJ3DP>WBDED>FDM, DIW >LOM According to the comparisons of each AM technique, DIW has the outstanding advantages in diversity in materials, low cost and also has competitiveness in speed. Particularly, diversity in materials make DIW as one of the most popular AM techniques. But DIW is not as good as VPP, PBF and IJP in resolution. Thus, DIW is often used in applications when printing resolution and surface roughness are not the primary concerns and as long as the prepared ink

resolution and surface roughness are not the primary concerns and as long as the prepared ink can possess specific rheological characteristics. Material currently suitable for DIW include polymer material, biological material, conductive metal material, cement, ceramic material and functional material. As shown in Figure 2.3, the application fields of DIW using the mentioned materials cover rubber engineering [62], tissue engineering [63], batteries [64], electronic circuits [65], buildings [66], ceramic engineering [67], sensors and 4D printing [68]. It is foreseeable that more and more new materials will be prepared as inks suitable for DIW and applied in more applications needing structural or functional materials or parts.



Figure 2.3 Suitable materials and corresponding applications for DIW: (a) polymer ink in rubber engineering[62]; (b) biological ink in tissue engineering[63];(c) metal ink in batteries[64], electronic circuits[65]; (d) cement ink in buildings[66];(e) ceramic ink in ceramic engineering[67]; (f) functional ink in 4D printing and sensors [68]

# 2.2.3 Development and challenges of DIW

# 2.2.3.1 Development of DIW

DIW, which is also named as Direct Write Fabrication [69] and Robocasting [70], was firstly proposed by Cesarano et al. in 1998 [71] and was patented in 2000 (US Patent: US6027326A) [72]. As shown in Figure 2.4 (a), The published patent describes the principle of DIW as: the ink is put into a syringe with a precision nozzle firstly; then, the ink is extruded to form extruded filaments and the nozzle is moved by computer control in a two dimensional (2D) pattern of each layer; finally, the nozzle is moved vertically and 3D parts are achieved by layer-by-layer accumulation. Further, the ink requirements are also illustrated in Figure 2.4 (b): (1) a shear thinning viscosity characteristic during extrusion to ensure good printability; (2) a good shape retention characteristic when stacked after extrusion. Figure 2.4 (c) shows the 3D parts constructed by DIW.



Figure 2.4 DIW technique proposed in the patent in 1998: (a) working principle, (b) ink requirements, (c) 3D parts constructed by DIW[72]

After the patent was disclosed, many research institutions discovered the obvious advantages of material compatibility, low cost and high efficiency of DIW compared with other AM techniques, and then carried out studies on material, process and applications for this technique. The more famous ones are Lewis Laboratory of Harvard University, DREAMS Lab of Virginia Tech, Manufacturing Processes and Machinery Lab of Washington State University, Swiss Federal Laboratories for Materials Science and Technology. Among them, the Lewis Lab of Harvard University has made the greatest contribution. Lewis Lab has been focusing on DIW since it was public. With more than 20 years of research, it has made significant contributions to its theoretical research, material preparation, process modeling, application and industrialization, which has greatly promoted the development and application of DIW. As shown in Figure 2.5, Lewis lab has firstly prepared new materials and pioneered the application in many new fields: in 2012, they prepared silk/hydroxyapatite(HA) ink for tissue engineering [73]; in 2013, they prepared lithium oxide ink for batteries [34]; in 2014, carbon ink was developed for electronics [74]; in 2015, wearable sensors were prepared using ion conductive ink [75]; in 2016, cellulose inks and polymer inks were prepared and were successfully applied to 4D printing [76] and soft robotics [77], respectively; in 2017, silver nano-ink was developed

for radio frequency devices [78]. The focus and key technology of Lewis Lab research is to analyze and control the rheological properties of ink, so that the filaments printed by DIW can be directly stacked layer by layer at room temperature and maintain good shape stability.



*Figure 2.5 Contributions of Lewis lab on DIW in recent years*[73], [34], [74], [75], [76], [77], [78]
Nowadays, with the development of DIW on materials, process and applications, DIW has become as one of the most popular AM techniques.

#### 2.2.3.2 Extrusion and deposition forms of DIW

#### (1) Extrusion methods

Extrusion methods of DIW include pneumatic force-driven, piston-driven and screwdriven (Figure 2.6). The ability to extrude the viscosity of the ink material is: pneumatic forcedriven<piston-driven</p>
screw-driven. Compared with the pneumatic force-driven and screwdriven DIW, piston-driven DIW has advantage in flow rate stability as the flow rate in pistondriven DIW is dependent only on the piston movement [79], which is of great benefit to the quality of printed parts [80].



Figure 2.6 There extrusion methods of DIW: pneumatic force-driven, piston-driven and screw-driven [81]

#### (2) Deposition forms

For ink deposition, two strategies are used according to self-support ability of inks in DIW [82] (Figure 2.7): the first one is to prepare high viscosity inks with shear-thinning and viscoelastic properties which can be extruded from a nozzle and have self-support ability after deposition to form 3D parts in room temperature directly (Figure 2.7 (a)) [83, 84]; the second one is to use assisted-deposition methods like UV-thermal curing (Figure 2.7 (b)) [85], suspended hydrogels (Figure 2.7 (c)) [86] or chemical process (Figure 2.7 (d)) [87] for inks with low viscosity and poor self-support ability. Compared with the low viscosity material based DIW with assisted-deposition systems, high viscosity material based DIW has advantage of low cost, high processing efficiency and high accuracy [88, 89]. Thus, due to the advantages of piston-driven extrusion method and direct deposition forming method based on high

viscosity material in DIW, high viscosity material based piston-driven DIW is the most popular choice in DIW. Thus, the term "DIW" in this thesis refers specifically to high viscosity material based piston-driven extrusion DIW.



Figure 2.7 Deposition strategies for DIW: (a) deposition directly; (b) deposition with UVthermal curing [85]; (c) deposition with suspended hydrogels [86]; (d) deposition with chemical process [87]

#### 2.2.3.3 Challenges and solutions of DIW

#### (1) Challenges of DIW

As a technique that has developed rapidly in recent years, although many scholars have done a lot of research on the development of DIW, there are still many challenges need to be solved to improve smooth surface finish, dimensional accuracy and properties (mechanical and functional) for the promotion and industrialization of DIW. The main challenges of DIW are summarized as follows [9]:

(1) Difficulty in building large overhangs or spans with perfect geometrical accuracy despite using ink with optimized rheology;

(2) Difficulty in ink preparation with optimized rheology: the ink needs to flow easily under shear stress and rapidly recovers and retains its shape upon deposition;

(3) Difficulty to extrude ink through extremely small to print high resolution parts as clogging;

(4) Difficulty to quickly find suitable process parameters for the prepared ink.

#### (2) Solutions of the challenges of DIW

Many scholars have done various research to come up with suggestions and references to solve the challenges. The solutions to the above challenges proposed by scholars are summarized as follows:

(1) For question (1), the researchers used sacrificial supports to grow the range of geometries that can be manufactured by the DIW [90];

(2) For question (2), the research hotspot mainly focus on the preparation of ink and then select the best ink using rheological characterization using rheology tests including shear stress ramp test, shear rate sweep test, frequency sweep test and recovery test [67];

(3) Question (3) can be avoided by using an appropriate surface lubricant such as oleic acid to reduces the friction between particles and agglomeration formation [91] and by improving nozzle designs [92];

(4) For question (4), scholars need to go through numerous trials to find a printable window of ink properties and process parameters suitable for DIW to obtain the printing quality that meets the requirements of use [15-17].

The main reason of question (4) is the research on the modelling and analysis of the DIW process is very lacking as the process modeling and analysis of DIW have not been fully studied, which limits the manufacturing accuracy and application promotion of this technique. The question largely increases cost and reduces application attractiveness of DIW. To solve this problem, it is critical to do research on process modeling and analysis for DIW.

#### 2.2.4 Discussion

Over the past five years, AM technology has gained a great attention and has been successfully used in various applications showing a great business potential. Owing to the outstanding advantages in diversity in materials and flexibility in equipment, DIW has become one of the most popular AM techniques and researchers have done numerous works on DIW for its application promotion. However, as a technique that has developed rapidly in recent years, there are still many challenges need to be solved for DIW. Specially, the research on the analysis of the DIW process is very lacking as the process modeling and analysis of DIW have not been fully studied, which limits the manufacturing accuracy and application promotion of this technique. To solve this problem, it is critical to do research on process modeling and analysis for DIW.

## 2.3 A literature review on process modeling and analysis for DIW

## 2.3.1 Input and output of process modeling for DIW

The purpose of process modeling for DIW is to construct the relationship between input and output in the printing process in order to predict the output according to the input before printing.

#### 2.3.1.1 Input of process modeling for DIW

For the input, the quality of DIW depends on the material properties of the ink including density, surface tension and viscosity [93-95] and the DIW process setting includes nozzle inner diameter, syringe diameter, piston speed, nozzle speed and layer height [96]. Thus, in process modeling for DIW, the inputs are the material properties of the ink and the printing process parameters setting (Figure 2.8).



Figure 2.8 Input and output of process modeling for DIW

#### 2.3.1.2 Output of process modeling for DIW

Firstly, Freeform extruded filaments (FEF) are extruded filaments in the air between the nozzle bottom and the substrate in DIW (Figure 2.9 (a)). During the DIW, producing continuous, tubular FEF with diameters close to the actual nozzle inner diameter is a prerequisite and also a characterization for a high printing quality [82]. For instance, Ouyang et al. [97] characterized ink printability through shape statuses of FEF as three status: "undergelation", "proper-gelation" and "over-gelation"; Paxton et al. [98] focused on the formation properties of FEF as an initial screening to assess ink printability; Smith et al. [82] proposed a term considering the measured diameter of the FEF and nozzle inner diameter to define printability; D ávila et al. [99] evaluated ink printability through observation of FEF formation; He et al. [100] chose suitable ranges for process parameters setting in DIW 3D printers by observing shapes of FEF. Therefore, FEF is one of the most basic output of process modeling for DIW and mean diameter and stability are two indicators to evaluate the FEF.

Secondly, FEF is deposited on the substrate forming as deposited filament (DF) (Figure 2.9 (b)). The quality of the DIW 3D printed parts depends on the deposition status and profile dimension of DF [101]. Kazemian et al. [102] proposed a real-time extrusion quality monitoring technique for cement ink based DIW by observing DF using computer vision. Tu et al. [103] divided the deposition status into "over-deposition", "pressed-deposition" and "freeform-deposition" based on the shapes of DF. Thus, DF is also one of the most basic output of process modeling for DIW and flow rate, deposition status, height and width are critical indicators for DF.

Thirdly, from DF to a layer, DF needs to change direction and deposited corners are formed (Figure 2.9 (c)). The geometrical quality of 3D parts fabricated by DIW is influenced by the deposition quality of deposited corners [104]. Several scholars have done researches on improving the geometrical quality of MEAM by controlling quality of deposited corners [105-108]. Akhoundi et al. [105] improved the quality of corners through printing speed optimization to realize high-quality printed composites with different geometric shapes for MEAM. Giberti et al. [106] presented a path planning technology to maintain a constant velocity along the trajectory in corners aimed at improving dimensional quality for MEAM. Jin et al. [107] proposed an optimized path planning technique to decrease the number of sharp corners in MEAM to improve deposition quality of printed parts. Li et al. [108] improved precision of deposited corners and parts of MEAM by in-situ monitoring and predicting 3D geometric

deviation. Thus, deposited corner is one of the most basic output of process modeling for DIW and corner angle and outline are elements of concern in process analysis for deposited corners.

Fourthly, a printed layer is deposited constructed by DF and deposited corners (Figure 2.9 (d)). Dimensional accuracy of printed layers could affect the whole part quality. At present, monitoring and control of printed layers is a research focus in AM quality control [109, 110]. He and Huang [111] predicted the in-plane shape of printed layers to improve the geometric accuracy of AM built products. He et al. [112] captured the image of each printed layer to control the whole process of FDM. Mohammad et al. [113] proposed a quality monitoring framework for 3D printing through monitoring each layer. Finally, a 3D part is printed by the layer-wise deposition (Figure 2.9 (e)). Thus, printed layer and 3D part are outputs of process modeling for DIW. For printed layers, the indicators include dimensional accuracy and roughness. For 3D parts, the indicators include dimensional accuracy, roughness, mechanical properties and functional properties.



Figure 2.9 Physical photos of outputs of process modeling for DIW: (a) FEF, (b) DF, (c) deposited corner, (d) printed layer, (e) 3D part

#### 2.3.2 Process modeling methods

Process modeling methods for MEAM include: analytical modeling methods [114], experimental data based modeling methods [115] and numerical simulation methods [116]. Each method is reviewed as follows.

#### 2.3.2.1 Analytical modeling methods

Analytical modeling methods give a process model based on the mathematical description and derivation of physical process. Owing to the quickness and simplicity of the analytical modeling methods in the modeling of the flow rate of DF in DIW, many scholars have established models of the flow rate for the pneumatic force-driven DIW through the analytical modeling methods [117-120]. However, few works gave the complete mathematical description for flow rate of piston driven DIW. Meanwhile, analytical modeling methods are currently applied to obtain flow dynamics parameters such as extrusion rate, shear stress, and real-time viscosity during DIW but it is difficult to obtain shape of DF, printed layers and 3D parts directly. Some scholars also give mathematical descriptions of shape of DF using analytical modeling method with approximation assumptions in the derivation [121, 122]. For example, Vlasea et al. [123] described an analytical model for line width of DF by simplifying the DF's cross-sectional profile as an elliptical segment. Lee et al. [121] developed a model for DIW to predict the width of DF with an equation describing the DF's area of a half-ellipse. Suntornnond et al. [122] proposed a mathematical model to predict the width of DF by assuming the DF's cross-sectional profile was circular. Haghbin et al. [124] predicted the sizes of DF using three geometric models of rectangle, oblong and ellipse for material extrusionbased 3D printing. All these studies established analytical models of the DF by first assuming that the cross-sectionals of DF were constant shapes and the shapes were simplified as circle, half-ellipse, ellipse, rectangle or oblong. However, cross-sectional shapes of DF will change under different conditions of inks and process parameters [125]. Thus, the simplification in analytical modeling of DF limited the model prediction accuracy in profile dimensions' prediction.

#### 2.3.2.2 Experimental data based modeling methods

Experimental data based modeling methods obtain data by using design of experiments (DOE) and obtain the model of DIW based on experimental data, which can give an intuitive description of process parameters and final prediction results. The main experimental data based modeling methods for AM include: Taguchi method [126], response surface methodology (RSM) [127] and machine learning (ML) method [128].

#### (1) Taguchi method

The Taguchi method was proposed by Dr. Genichi Taguchi in Japan. The purpose of Taguchi method is to obtain the optimal process parameters with the least test time and cost through DOE and to determine the contribution of each process parameter by analysis of variance (ANOVA) [129]. The Taguchi method uses "signal" and "noise" to represent the expected value (mean value) and unexpected value (variance), respectively, and uses the signal-to-noise ratio (SNR) as an indicator for quality. Because the Taguchi method has the characteristics of minimizing the test cost, it has been widely used in the process parameter optimization and process modeling of MEAM. For example, Namsoo et al. [130] used the Taguchi method to optimize the process parameters of screw extrusion 3D printing process; Emily et al. [131] used the Taguchi method to analyze the influence of parameters including printing temperature, post-processing temperature and post-processing time on the strength of parts obtained by extrusion based 3D printing and to select the optimal process parameters setting; Ala'aldin et al. [132] used the Taguchi method to analyze the impact of various parameters including filling ratio, filling pattern, layer thickness and extrusion temperature on the mechanical strength and dimensional accuracy of products in extrusion based 3D printing.

#### (2) Response surface methodology (RSM)

The purpose of RSM is to obtain an intuitive graphical optimization area through DOE and data analysis. Firstly, experimental data are obtained through DOE. Then, functional relationship between process parameters and target responses is obtained using data fitting. Finally, the functional relationship is used to guide the multi-optimization problem to find the optimal process parameters [133]. At present, RSM is widely used in the field of process parameters optimization for manufacturing [134, 135].

#### (3) Machine learning (ML) method

The ML method is an advanced method based on artificial intelligence that can perform pattern recognition from complex data sets [136] with the advantage of not requiring complex process analysis. According to the learning method, ML methods can be divided into supervised learning, unsupervised learning and reinforcement learning.

#### **Supervised learning**

Supervised learning uses a computer program to learn from a set of labeled data in a training set to identify unlabeled data from a test set with the highest accuracy. The purpose of supervised learning is to obtain the relationship between data from the data set through computer programs, so as to predict the corresponding labels for new feature data without

labels [137]. Commonly used supervised learning algorithms include linear regression algorithm, polynomial regression, decision tree, random forest, support vector machine, artificial neural network, convolutional neural network, and recurrent neural network [138].

#### **Unsupervised learning**

Unsupervised learning infers from unlabeled data [139], which is a data-driven ML method that can discover patterns or groupings hidden by similar data (i.e., clusters) in a given random dataset. Unsupervised learning is widely used in anomaly detection [140], recommender systems [141] and market classification [142]. Commonly used unsupervised learning algorithms include K-means algorithm and K-medoids algorithm.

#### **Reinforcement learning**

Reinforcement learning is a semi-supervised form of ML that allows the model to interact with the environment and learn to take the best actions that will yield the greatest reward. It does not require a training dataset and the model learns from its own actions. Reinforcement learning is currently widely used in robotic arms [143], self-driving cars [144] and AlphaGo [145]. Commonly used reinforcement learning algorithms include Q-learning algorithm, deep Q-learning algorithm, deterministic policy gradient algorithm, and deep deterministic policy gradient algorithm.

However, the disadvantage of the ML method is that it requires a large amount of data sets, additional material/time consumption and computing resources.

#### (4) Limitations of experimental data-based modeling methods

In summary, experimental data-based modeling methods including Taguchi method, RSM and ML methods have been widely used in manufacturing process modeling. However, these methods are limited by the experimental equipment. Some parameters are not easy to measure in DIW directly such as the speed of extruded filaments. At the same time, the model constructed by this method usually does not contain time parameter which results that it cannot be used for prediction in real time. Finally, the method requires extensive experimentation, time, material and cost.

#### 2.3.2.3 Numerical simulation methods

As an important supplement to analytical modeling methods and experimental data based modeling methods, numerical simulation methods can provide a large amount of information on the AM process and has been widely used in the process modeling and analysis of MEAM. For example, Liravi et al. [146] used finite element analysis (FEA) to establish a model of high-viscosity material flow during extrusion 3D printing; G öhl et al. [147] used computational fluid

dynamics (CFD) software IPS IBOFlow to predict ink printability in DIW; Balani et al. [148] used numerical simulation to determine the velocity profile, shear force and real-time viscosity of PLA material in FDM; Liu et al. [149] used numerical simulation to evaluate the dynamic process of FDM; Comminalet al. used numerical simulation methods to conduct extensive modeling studies on MEAM, including simulation modeling of extrusion of high-viscosity materials [150], CFD simulation modeling of extrusion filament deposited on the substrate [151], simulation modeling of extrusion filament corners [152] and simulation modeling of polymer material flow in the nozzle [153].

The most commonly used numerical simulation methods are: volume of fluid (VOF) method [154], level set method [155], phase field method [156], lattice Boltzmann method [157] and direct interface tracking method [158]. The idea of VOF method is to introduce the volume fraction and treat the two-phase flow as a single flow model with variable material properties including density and viscosity. And then VOF uses the volume fraction to determine the position of the liquid free surface. The idea of the level set method is to regard the tracked moving interface as the zero isosurface of the level set function and extend the velocity of the interface to the level set function, and obtain the position of the fluid interface by solving the level set function. The idea of the phase field method is to use a very thin finite thickness to represent the phase interface and the state parameters on the interface are continuously distributed and have a high gradient. The idea of the lattice Boltzmann method is to simulate fluid flow at the mesoscopic scale by solving the discrete Boltzmann equation. The direct interface tracking method defines the marker variables of the two-phase flow interface position and uses a fixed grid in the entire flow field; finally, the position and shape of the twophase flow interface at each moment is tracked by solving the governing equations on the fixed grid. Among these methods, VOF method is currently the most commonly used method for process modeling of MEAM process due to its simplicity, robustness, and accuracy [159, 160].

Numerical simulation is one of the most powerful tools in process modeling analysis in AM. Process analysis based on numerical simulations has advantages in saving material/trial time and easily capturing critical process parameters value which are difficult obtained by experimental measurements. Although a large number of studies have used numerical simulation modeling methods to establish process models of MEAM, there is currently few systematic works on process modeling and analysis based on numerical simulations for DIW. Thus, to improve the manufacturing accuracy and application promotion of DIW, it is

meaningful and critical to do research on process modeling and analysis based on numerical simulations for DIW.

### 2.3.3 Conclusion

The purpose of process modeling for DIW is to construct the relationship between inputs and outputs in the printing process, which is used to predict the outputs according to the inputs before printing. The inputs are summarized as the material properties of the ink (density, surface tension and viscosity) and the printing process parameters setting (nozzle inner diameter, piston diameter, piston speed, nozzle piston, layer height). The outputs include the FEF, DF, deposited corner, printed layer and 3D part. Numerical simulation is one of the most powerful tools in process analysis in AM. Process analysis based on numerical simulations has advantages in saving material/trial time and easily capturing critical process parameters value which are difficult obtained by experimental measurements. The research on process modeling and analysis of DIW based on numerical simulations will provide important support for the development and guidance of DIW. However, the literature review shows that there is currently few systematic works on process modeling and analysis based on numerical simulations for DIW. To bridge this gap, the objective of this thesis is to do research on process modeling and analysis for DIW based on numerical simulations. The next two chapters describe in detail the proposed numerical approach and its results.

## Chapter 3: Ink material properties characterization and process parameters selection

## **3.1 Introduction**

The printing quality of DIW process depends on ink material properties and process parameters setting. Recent studies [93-95] focused on inks preparation and ink material properties characterization as ink material properties play the most critical role in extrusion process, shrinkage, shape fidelity and structural stability. DIW process parameters concerned with the equipment considerably affect the parts' dimensional accuracy [96]. Meanwhile, ink material properties and process parameters are inputs of process modelling of DIW. Thus, this chapter presents our research work on ink material properties characterization and process parameters selection to provide the basis for modeling inputs of DIW.

For ink material properties characterization, density, surface tension, static contact angle and rheology properties are obtained for the used ink through experimental methods.

For process parameters selection. Recently, the selection of process parameters for DIW has been conducted by many scholars [98, 161, 162]. However, all these studies just determined a printability window instead of an optimal value and few studies are available for process parameters significance analysis and optimization for DIW. Therefore, it is imperative to investigate the significance of each process parameter and find optimal process parameters setting to improve dimensional accuracy of parts in DIW.

Taguchi method [126] and machine learning (ML) methods [108, 163] have been widely used to control process parameters of material extrusion-based 3D printing. ML methods enable the proper parameters selection with little process analyses but need large dataset, additional time and computing resources [136]. Taguchi technique is more efficient [164] with a significant slash in experimental time and cost [129] and it can determine the significance of each parameter by analysis of variance (ANOVA) [165]. To perform DIW process parameters optimization with minimum material and time, Taguchi method is adopted in this chapter.

This chapter starts with the presentation of ink material properties characterized for the used ink in this thesis. Then, process parameters are selected for the used ink in the DIW 3D printer. Especially, in process parameters selection, we identify DIW process parameters

through printing analyses and propose a two-step optimization method to optimize DIW process parameters for dimensional accuracy of printed layers and analyze the significance of each process parameter. To verify the method, confirmation tests are conducted considering the condition comparison and the method robustness on other shapes as well as parameter adaptability in 3D parts printing from printed layers' analyses for the proposed method and parameter adaptability in constructs fabricated as 100% infill or with porosities.

## **3.2 Ink properties characterization**

#### 3.2.1 Ink used in this thesis

The objective of this thesis is to develop an approach on process modeling and analysis for DIW based on numerical simulations. Ink preparation is not research content in this thesis. Thus, a well-printable ink is selected and used directly in this thesis.

Nivea Cr ème (Art. No. 80104) (Beiersdorf Global AG, Germany) is chosen as the ink reference material to verify the proposed numerical simulations because Nivea Cr ème is used as printability reference for inks to test the process parameters in DIW and can represent numerous printable inks in DIW [98]. Nivea Cr ème meets the requirements of DIW inks material properties (shear thinning ability during extrusion and shape retention after deposition) and many inks in DIW are designed and produced to have the same printability of Nivea Cr ème.

The main ingredients of the Nivea Crème include water, mineral oil, petrolatum, glycerin, microcrystalline wax, lanolin alcohol, paraffin, panthenol, magnesium sulfate, decyl oleate, octyldodecanol, aluminum searates, fragrance, citric acid, magnesium stearate, methylchloroisothiazolinone, methylisothiazolinone. Among these ingredients, water is solvent; glycerin is humectant; lanolin alcohol is emulsion stabilizer; microcrystalline wax is thickening agent and binder. And microcrystalline wax has the greatest effect on the rheological properties and printability of the Nivea Crème ink.

#### **3.2.2** Ink material properties characterization tests

#### 3.2.2.1 Density, surface tension, static contact angle

A 5 mL pycnometer and analytical balance XSR (both from Mettler Toledo, France) are used to assess ink density by measuring a mass of 5 mL of the ink (measuring accuracy: 0.008 mg).

A tensiometer K9 (KRÜSS, Germany) is used to measure the surface tension coefficient using the Du Noüy ring method (measuring accuracy: 0.1 mN/m).

Static contact angle is measurement by observing the cross-sectional profile of DF in DIW without stretch or squeeze using the method proposed in the paper [125]. In this method, a section of DF is printed in the steady-state coiling regime to ensure the DF is not stretched by the translational motion of the nozzle or not squeezed by over deposition of DF.

All measurements of density, surface tension and static contact angle are performed at 25 °C and repeated three times.

#### 3.2.2.2 Rheology characterization

A complete rheological characterization for Nivea Crème is conducted as ink rheology plays the most critical role in DIW. A rheometer ARES (TA Instruments, USA) with a 25 mm plate-plate geometry at a gap distance of 1 mm is used in ink rheology characterization. Especially, shear stress ramp test, shear rate sweep test, frequency sweep test and recovery test are conducted to determine yield stress, viscosity, modulus (including storage modulus (G') and loss modulus (G'')) and recovery characteristic, respectively. Shear stress ramp test and shear rate sweep test are used to characterize the shear-thinning rheology property of the ink. Frequency sweep test and recovery test are used to characterize the shape retention rheology property of the ink.

In shear stress ramp test, shear stress is changed from 2 Pa to 900 Pa and the shear stress are set to 10 points evenly distributed within 100 Pa. In shear rate sweep test, shear rate is changed from 0.0125 to 100  $s^{-1}$  and the shear rates are set to 5 points per decade. In frequency sweep test, angular frequency is changed from 100 rad/s to 1 rad/s in 1rad/s interval. In recovery test, from 0-200 s, the shear rate value is set as 0.0125  $s^{-1}$ ; from 200-300 s, the shear rate value is set as 895  $s^{-1}$ ; from 300-500 s, the shear rate value is set as 0.0125  $s^{-1}$ . All measurements are performed at 25 °C and repeated three times.

The Hershel-Bulkley model (HBM) has been verified and adopted as a suitable and reliable model to represent the viscosity of the inks in DIW with shear-thinning and shape retention rheology property [161, 166]. Using the HBM, the shear stress and the viscosity of inks can be expressed by Eq. (3.1) and Eq. (3.2), respectively.

$$\tau = \tau_0 + K \mathcal{R} \tag{3.1}$$

$$\mu = \min\left(\mu_0, \tau_0 / p^{\mathbf{k}_{+}} K p^{\mathbf{k}_{-1}}\right) \tag{3.2}$$

Where  $\tau$  (unit: *Pa*),  $\not\approx$  (unit: *s*<sup>-1</sup>),  $\mu$  (unit: *Pa*·*s*) are variables named as shear stress, shear rate, dynamic viscosity for inks in flow;  $\mu_0$  (unit: *Pa*·*s*),  $\tau_0$  (unit: *Pa*), *K* (unit: *Pa*·*s*<sup>*n*</sup>), *n* (unit: dimensionless) are rheological properties called as limiting dynamic viscosity, yield

stress, consistency index, flow index for inks. If stress  $< \tau_0$ , the ink behaves as a rigid solid, otherwise it behaves as a fluid. For n < 1, the ink is shear-thinning, whereas the ink is shear-thickening. A large  $\mu_0$  means that the ink will only flow in response to a large applied force.

 $\mu_0$  and  $\tau_0$  are determined using experimental viscosity-shear stress curve obtained by shear stress ramp test: abscissa and ordinate of intersection point between two linear regressions at the plateau-region and viscosity-drop regions of the viscosity-shear stress diagrams are  $\mu_0$  and  $\tau_0$ , respectively. *K* and *n* are determined through regression between Eq. (3.2) and experimental viscosity-shear rate data obtained by shear rate sweep test.

#### 3.2.3 Ink material properties characterization results

#### 3.2.3.1 Results of density, surface tension, static contact angle

The density and surface tension coefficient of the Nivea Crème are obtained by density and surface tension tests and the results are: density  $\rho$  is 972  $k_g/m^3$  and surface tension coefficient  $\sigma$  is 43 mN/m.

For static contact angle, as shown in Figure 3.1 (a), a section of filament is printed in the steady-state coiling regime which ensured the filament is not stretched by the translational motion of the nozzle. As shown in Figure 3.1 (b), static contact angle  $\theta_c$  is measured directly through photo of cross-sectional profile of the filament and the value of  $\theta_c$  is 180 °.



Figure 3.1 Experimental results of static contact angle of the Nivea Cràne: (a) top view of filament printed in the steady-state coiling regime, (b) cross-sectional profile of the filament

#### 3.2.3.2 Results of rheology characterization

Results of rheology characterization are plotted in Figure 3.2. The result shear stress ramp test (Figure 3.2 (a)) shows that the ink stays rest when the shear stress value is below yield

stress and starts to flow when the shear stress value exceeds yield stress. Figure 3.2 (b) shows the shear-thinning characterization of the ink as viscosity decreases with the increase of shear rate. The ink exhibits a solid-like response as its storage modulus (G') exceeds its loss modulus (G'') (Figure 3.2 (c)), which means the ink has low shrinkage and good shape fidelity. Moreover, the structural stability of the ink is also good as shown in Figure 3.2 (d): from 0-200 s, the viscosity stays stable and in high value when shear rate value is near 0; from 200-300 s, the viscosity stays stable and in low value when shear rate value is  $895 \ s^{-1}$ ; from 300-500 s, the shear rate value recoveries to near 0 and the viscosity recoveries to stay stable and in high value. In conclusion, Nivea Cr ème is verified as a well-printable ink through the rheological characterization.

Then, parameters in HBM viscosity model are obtained through data analyses of Figure 3.2 (a) and Figure 3.2 (b). As shown in Figure 3.2 (a),  $\mu_0$  and  $\tau_0$  are determined using the intersection point of two tangents in the diagram of shear stress ramp test data where one is stable platform line (red dotted line) in the plateau-region and the other one is the quickly-drop line (purple dotted line) in the viscosity-drop region. Abscissa and ordinate of the intersection point are  $\mu_0$  and  $\tau_0$ , respectively. The results are:  $\mu_0 = 1.58 \times 10^6 Pa \cdot s$ ;  $\tau_0 = 563 Pa$ .

As shown in Figure 3.2 (b), shear thinning parameters, *K* and *n*, are obtained by fitting Eq. (3.2) with the viscosity-shear rate data using data regression. The results are:  $K = 867 \ Pa \cdot s^n$ ; n = 0.045. The coefficient of determination ( $R^2$ ) and p-value of fitting results are 0.9947 and 0.0000<0.05, verified the fitting results is correct.

In conclusion, results of ink material properties are all obtained and listed in Table 3.1.

Parameter	Density p (kg/m <sup>3</sup> )	Surface tension coefficient $\sigma$ (mN/m)	Static contact angle $\theta c$ ( )	Limiting dynamic viscosity $\mu_0$ (Pa.s)	Yield stress $\tau_0$ (Pa)	Consistency index K (Pa.s <sup>n</sup> )	Flow index n
Value	972	43	180	1.58×10 <sup>6</sup>	563	867	0.045

Table 3.1 Ink material properties of the selected ink Nivea Crème



Figure 3.2 Rheological characterization of Nivea Cr àme (Art. No. 80104): (a) limiting dynamic viscosity and yield stress determination through shear stress ramp test; (b) viscosity as a function of shear rate; (c) storage (G') and loss (G'') modulus as a function of frequency; (d) stability analysis through recovery test

## 3.3 Process parameters selection

## 3.3.1 DIW 3D printer used in this thesis

A piston driven DIW 3D printer TM-081 (Tobeca Company, France) is used in this thesis as illustrated in Figure 3.3 (a). The piston movement is driven by a mechanical system, which extrudes out ink in the syringe through the nozzle into the air and finally on the substrate. Then, a three-axis movement frame guides the nozzle to move in x and y directions to deposit the extruded filaments on a planar region as nozzle is fixed in z direction. Afterward, the nozzle moves to the next layer and 3D parts are printed layer by layer.



Figure 3.3 Process parameters identification for DIW process: (a) the DIW 3D printer used in this thesis; (b) the DIW process; (c) process parameters setting in Step 1

#### **3.3.2 Identification of process parameters**

Process parameters are identified through DIW process analysis. As shown in Figure 3.3 (b), DIW process for a printed layer includes two steps. Step 1 is to print a line by moving nozzle from point A to point B. Then, a layer is printed by arranging lines tightly in Step 2. Thus, DIW process parameters for printed layers are divided into two categories as:

- 1) Process parameters for printing a line;
- 2) Extra process parameter from lines to a layer.

#### 3.3.2.1 Process parameters for printing a line

The process parameters for printing a line is illustrated in Figure 3.3 (c). Piston diameter  $D_p$  and inner diameter of nozzle  $d_n$  are dependent on equipment and considered as constants. Their values are 21.6 mm and 0.84 mm, respectively.  $v_p$  (piston velocity),  $v_n$  (nozzle velocity) and h (gap between nozzle bottom surface and substrate) are identified as controllable process parameters.  $v_e$  (average velocity of extruded filament on the nozzle bottom surface), which is dependent on  $v_p$  and equipment, is uncontrolled process parameters.

In extrusion-based AM, optimal  $v_n$  depends on  $v_p$  [152] and optimal h depends on  $d_n$  [150]. If  $v_p$ ,  $v_n$  and h are set independently without regard to the relationship between these parameters, the optimization would be inefficient and even incorrect. Thus, process parameters for printing a line are identified as:  $v_n$ ,  $V^*$  (dimensionless nozzle velocity, defined as  $v_n/v_e$ ) and  $H^*$  (dimensionless height, defined as  $h/D_p$ ). Because the ink extrusion and deposition process are considered as an isothermal, incompressible and laminar flow, the average velocity

on each cross section in the nozzle is the same and  $v_e$  can be expressed as follows using conservation of mass.

$$v_e = \left(D_p / d_n\right)^2 v_p \tag{3.3}$$

#### 3.3.2.2 Extra process parameter from lines to a layer

As illustrated in Figure 3.3 (b),  $\overline{w}_o$  (average width of the optimal printed line) of printed line under optimal condition is measured in Step 1. Then, a rectangular object (reprehensive of the printed layers) is printed by controlling  $d_i$  (distance between lines) line by line. In extrusion-based AM, optimal  $d_i$  depends on  $\overline{w}_o$  [151]. Thus, extra process parameter from lines to a layer is identified as  $R_w$  (ratio of  $d_i$  to  $\overline{w}_o$ ) and  $d_i$  could be determined as follows:

$$d_l = R_W \cdot \bar{w}_o \,. \tag{3.4}$$

 $R_W$  mainly reflects the impact of W (the weight of the printed layer) on distortion in x-y plane (detailed relationship between  $R_W$  and W as well as its derivation process are shown in the Appendix A of Appendices).

Consequently, DIW process parameters are identified as:

- 1) Process parameters for printing a line:  $v_n$ ,  $V^*$  and  $H^*$ ;
- 2) Extra process parameter from lines to a layer:  $R_{\rm w}$ .

#### **3.3.3 Definition and measurement method of dimensional errors**

Dimensional errors are divided into dimensional error for printed lines and dimensional error for printed layers according to the two categories of identified process parameters. x-y plane dimensional accuracy is of primary interest and dimensional accuracy in the z axis can be ignored for layer accuracy analyses because previous studies [109, 111, 113] have verified that the use of control charts with image data only considering x-y plane dimensions for each layer could improve quality of parts in 3D printing significantly.

### 3.3.3.1 Dimensional error for printed lines and its measurement method

#### (1) Definition of dimensional error for printed lines

As illustrated in Figure 3.4 (a),  $N_1$  measuring points are set along the line length uniformly and widths of line on each measuring point are measured as  $w_i$  ( $i = 1, 2, ..., N_1$ ). Average width of the printed line is calculated as follows:

$$\bar{w} = \sum_{i=1}^{N_1} w_i / N_1 \,. \tag{3.5}$$

Because the designed dimension of line is not specified and the most concerned quality of the printed lines is stability, which means the line width need to be always same along the deposition direction, the referenced dimension of line is defined as the average width  $\bar{w}$  and the dimensional errors  $el_i(i = 1, 2, ..., N_1)$  on each measuring point along length are defined as follows:

$$el_i = w_i - \overline{w}, (i = 1, 2, ..., N_1)$$
 (3.6)



Figure 3.4 Definition and measurement method of dimensional errors: (a) definition of dimensional errors for printed lines; (b) measuring points setting for printed lines; (c) definition of dimensional errors for printed rectangular objects; (d) measuring points setting for printed rectangular objects

#### (2) Measurement method of dimensional error for printed lines

As shown in Figure 3.4 (b), to reduce measurement error and consider the printing stability in the whole range, three lines are printed (each line is 100 mm long) and 9 measuring points are set for each line uniformly. 27 measuring points are uniformly distributed along lines as  $w_1$ to  $w_{27}$ . Minimum and maximum widths of lines except 27 measuring points are measured as  $w_{28}$  and  $w_{29}$ . Thus, totally 29 dimensional errors are used for dimensional accuracy analysis of printed lines. In practice, a ruler is put beside printed lines as reference dimension and photo of printed lines with ruler is taken using a camera (Canon LEGRIA HF R86 Noir, Canon Inc., Japan). Then, photo is imported into MATLAB and widths are measured using virtual ruler of the graphic processing tools in MATLAB.

#### 3.3.3.2 Dimensional error for printed rectangular objects and its measurement method

#### (1) Definition of dimensional error for printed rectangular objects

As illustrated in Figure 3.4 (c),  $N_2$  and  $N_3$  measuring points are set along x and y directions in the printed rectangular object uniformly and lengths on each measuring point along x and y direction are measured as  $lx_i$  ( $i = 1, 2, ..., N_2$ ) and  $ly_i$  ( $i = 1, 2, ..., N_3$ ). Average lengths for x and y directions are calculated as follows:

$$\bar{l}x = \sum_{i=1}^{N_2} lx_i / N_2$$
(3.7)

$$\bar{l}y = \sum_{i=1}^{N_3} ly_i / N_3$$
(3.8)

Designed dimensions for rectangular object in x and y directions are Lx and Ly. Dimensional errors for the printed rectangular object in x and y directions are defined as follows:

$$erx_i = lx_i - Lx, (i = 1, 2, ..., N_2)$$
 (3.9)

$$ery_i = ly_i - Ly_i (i = 1, 2, ..., N_3)$$
 (3.10)

#### (2) Measurement method of dimensional error for printed rectangular objects

To reduce measurement error and consider the printing stability in the whole range, measuring points setting for printed rectangular objects are shown in Figure 3.4 (d). Designed dimensions for rectangular object in x and y directions are Lx = 30 mm and Ly = 20 mm, respectively. In x direction, 10 measuring points are set uniformly as  $lx_1$  to  $lx_{10}$ . Minimum and maximum lengths except 10 points are measured as  $lx_{11}$  and  $lx_{12}$ . In y direction, 8 measuring points are set uniformly as  $ly_1$  to  $ly_8$ , and minimum and maximum lengths except 8 points are measured as  $ly_9$  and  $ly_{10}$ . Thus, 12 lengths are measured in x direction as  $lx_1$  to  $lx_{12}$ ; and 10 lengths are measured in y direction as  $ly_1$  to  $ly_{10}$ . Totally, 22 dimensional errors are used for dimensional accuracy analysis of printed rectangular objects. In practice, the lengths measurement method is same as widths measurement for printed lines using ruler beside the printed object and MATLAB.

# **3.3.4 Framework for DIW process optimization and orthogonal array** selection procedure

#### 3.3.4.1 Framework for DIW process optimization

The framework of DIW process optimization contains two steps and the two-step process parameters optimization method is shown in Figure 3.5. Step 1 is to optimize process parameters for printing a line. In step 1, continuity and uniformity of FEF and DF and printed rectangular objects on the substrate are observed in screening experiments to determine printability windows for each process parameter. Then, interaction effect tests are conducted and design of freedom (DOF) for experiments is calculated followed by orthogonal array (OA) selection for Taguchi design. Next, main experiments of line printing based on Taguchi method are conducted. SNR calculations and ANOVA are performed for Taguchi method based data to find the optimal combination and evaluate the significance respectively. Step 2 is to optimize extra process parameter from lines to a layer. In Step 2, the average width of printed lines under optimal condition is obtained firstly. Then, single-factor tests of rectangular object printing are conducted to find the optimal  $R_w$ . Finally, the optimal combination of total identified process parameters is summarized through step 1 and step 2 of the framework.



Figure 3.5 Framework of the proposed two-step method for optimizing DIW process parameters for printed layers

#### 3.3.4.2 Orthogonal array (OA) selection procedure

Instead of conducting full factorial experiments, Taguchi method based experiments of different process conditions are conducted through an OA, minimizing the number of experiments while ensuring the validity and robustness of the data [167]. The OA is selected based on DOF calculation considering the number of factors, interactions between them and the number of levels of each factor [168]. The procedure for OA selection is as follows:

(1) Determine the number, levels and interaction effects of factors.

(2) Calculate the total DOF of factors. DOF for a single factor is equal to one less than the number of levels of that factor. DOF for a two-factor interaction effect is equal to  $(S_1-1)\times(S_2-1)$  as  $S_1$  and  $S_2$  are DOF of the two factors. Total DOF of factors is cumulative sum of DOF of all single factors and DOF of all two-factor interaction effects.

(3) OA is selected from commonly used standard OAs based on total DOF of factors as number of experiments should require Eq. (3.11) as follows [169]:

$$T \ge DOF_{total} + 1 \tag{3.11}$$

Where T is number of experiments;  $DOF_{total}$  is total DOF of factors and their interaction effects.

## **3.4 Process parameters selection results**

## 3.4.1 Optimization of printed line

#### **3.4.1.1 Printability windows**

The term 'printability window' is defined as the combination of process parameters required for successful extrusion for DIW [98]. In experiments, printability window determination criterions include three points: continuity and uniformity of 1) FEF; 2) DF and 3) printed rectangular object on the substrate.

In screening experiments of FEF,  $v_p$  is calculated using Eq. (3.3) by fixing  $V^*$  as 1 and changing  $v_n$  from 1 mm/s to 20 mm/s (interval is 2 mm/s). In screening experiments of DF,  $v_n$  is fixed in printability window; then  $V^*$  is changing from 0.2 to 1.2 (interval is 0.2) and  $H^*$  is changing from 0.2 to 1.2 (interval is 0.1), respectively. In screening experiments of printed rectangular objects on the substrate,  $v_n$ ,  $V^*$  and  $H^*$  are fixed in printability window; and  $R_w$  is changing from 0.2 to 1 (interval is 0.1).

Through screening experiments, printability windows of each process parameter for the prepared ink are listed as:  $(5\sim11)$  mm/s for  $v_n$ ;  $(0.6\sim1)$  for  $V^*$ ;  $(0.6\sim1.2)$  for  $H^*$  and  $(0.5\sim0.9)$  for  $R_w$ .

#### 3.4.1.2 Orthogonal array (OA) selection

The lower value, middle value and higher value of printability windows for each factor in step 1 ( $v_n$ ,  $V^*$  and  $H^*$ ) are considered to be level 1, 2 and 3 respectively as listed in Table 3.2.

Parameter	Range	Level 1	Level 2	Level 3
$v_n$	(5~11) mm/s	5	8	11
$V^*$	0.6~1	0.6	0.8	1
$H^*$	0.6~1.2	0.6	0.9	1.2

Table 3.2 Levels of process parameters in step 1

In this step, two-factor interaction effects are considered. In interaction effect tests, one factor of  $v_n$ ,  $V^*$  and  $H^*$  is fixed and the remaining two factors are changed to print lines for

interaction effect analysis of the remaining two factors. Average widths of printed lines under each process parameters setting are calculated as indicator to analyze interaction effects. Interaction effect graphs are plotted in Figure 3.6 (a) (detailed information of interaction effect tests is summarized in the Appendix B of Appendices).



Figure 3.6 (a) Interaction effect graphs of step1 for: (a.1)  $v_n \times V^*$ ; (a.2)  $v_n \times H^*$ ; (a.3)  $V^* \times H^*$ and (b) mean SNR graph for main experiments in step 1

Interaction effect graph is a tool to study whether influence of one factor affects the function of the other factors [170]. In the graph, parallel line shows no interaction effect and the intersect or intersect trend between lines means a high degree of interaction [171]. As illustrated in Figure 3.6 (a), interaction effects of  $v_n \times V^*$ ,  $v_n \times H^*$  and  $V^* \times H^*$  should be considered as two lines in graphs intersect for  $v_n \times V^*$  as well as  $v_n \times H^*$  and had intersect trend for  $V^* \times H^*$ . Thus, three factors  $(v_n, V^* \text{ and } H^*)$  and three interaction effects  $(v_n \times V^*, v_n \times H^*$  and  $V^* \times V^*$ ,  $v_n \times H^*$  and  $V^* \times H^*$ .

DOF of single factor and their interaction effects are calculated according to Section 3.3.4.2 and the calculation result of total DOF of factors is 21. Thus, according to Eq. (3.11),  $L_{27}$  OA ( $L_T$  means OA with *T* experiments) is selected for main experiments of step 1 as shown in Table 3.3, from commonly used standard OAs for three-level Taguchi design including  $L_9$ ,  $L_{18}$  and  $L_{27}$ .

	Experimental	condition		
Experiment number	$v_n/(\text{ mm/s})$	$V^*$	$H^{*}$	SNR of dimensional errors
N1	5	1	0.6	22.51
N2	5	1	0.9	27.14
N3	5	1	1.2	22.73
N4	5	0.8	0.6	24.36
N5	5	0.8	0.9	36.83
N6	5	0.8	1.2	33.42
N7	5	0.6	0.6	29.24
N8	5	0.6	0.9	30.33
N9	5	0.6	1.2	32.41
N10	8	1	0.6	23.80
N11	8	1	0.9	22.40
N12	8	1	1.2	22.07
N13	8	0.8	0.6	37.32
N14	8	0.8	0.9	33.76
N15	8	0.8	1.2	25.78
N16	8	0.6	0.6	23.53
N17	8	0.6	0.9	25.37
N18	8	0.6	1.2	23.45
N19	11	1	0.6	36.61
N20	11	1	0.9	24.71
N21	11	1	1.2	23.74
N22	11	0.8	0.6	27.22
N23	11	0.8	0.9	26.96
N24	11	0.8	1.2	25.94
N25	11	0.6	0.6	26.78
N26	11	0.6	0.9	28.56
N27	11	0.6	1.2	26.52

Table 3.3 Experimental plan and calculated SNR for main experiments of step 1

#### 3.4.1.3 SNR analysis

Main experiments of step 1, containing 27 experimental runs, are conducted as shown in Table 3.3. Based on the requirements of response, SNR is divided into three categories namely medium-the-better, higher-the-better and lower-the-better [172]. In optimization of printed lines, the dimensional error is the lower-the-better to enhance the printing accuracy. Hence, Eq. (3.12) is used to calculate the SNR; and results are listed in Table 3.3.

$$\eta = -10 \log \left( \frac{1}{N_m} \sum_{i=1}^{N_m} y_i^2 \right)$$
(3.12)

Where  $\eta$  is the average SNR,  $N_m$  is the number of experiments conducted at level *i* and  $y_i$  is the evaluation value (dimensional error).

The mean SNR response of each process parameters in each level is calculated and listed in Table 3.4. Figure 3.6 (b) represents the mean SNR graph. Higher SNR represents the minimum variation difference between the desired output and evaluated output. Therefore, optimal process parameters for high dimensional accuracy using Taguchi method are found as:  $v_n = 5 \text{ mm/s}, V^* = 0.8, H^* = 0.9.$ 

Process	Mean SNR for	dimensional error	Max-Min	Rank	
parameters	Level 1	Level 2	Level 3		Kulik
<i>V</i> <sub>n</sub>	28.77	26.38	27.45	2.39	2
$V^*$	27.35	30.18	25.08	5.10	1
$H^{*}$	27.93	28.45	26.23	2.22	3

Table 3.4 Mean SNR response table for dimensional error of main experiments in step 1

#### **3.4.1.4 ANOVA results**

ANOVA is a tool to investigate the significant effect and indicate the contribution of process parameters in machinability researches [173]. ANOVA results for dimensional error of printed lines obtained using Minitab software is shown in Table 3.5. From Table 3.5, it is found that dimensional error is significantly influenced by  $v^*$  followed by  $v_n \times V^*$ ,  $v_n \times H^*$ ,  $H^*$ ,  $v_n$  and  $V^* \times H^*$ . The contribution percentages of process parameters setting for  $v^*$ ,  $H^*$  and  $v_n$  on dimensional error are 27.78%, 6.64% and 6.37%, respectively, meaning  $V^*$  is the most important process parameters for dimensional error of printed lines for the selected ink. Meanwhile, interaction effects of  $v_n \times V^*$ ,  $v_n \times H^*$  and  $V^* \times H^*$  influenced dimensional error in

26.65%, 7.01% and 4.41% percentage of contribution respectively. Thus, OA selection for Taguchi design should consider interaction effects of  $v_n \times V^*$ ,  $v_n \times H^*$  and  $V^* \times H^*$  as interaction effects of  $v_n \times V^*$ ,  $v_n \times H^*$  and  $V^* \times H^*$  and  $V^* \times H^*$  have big influences on dimensional error.  $V^*$  is highly significant in dimensional error at 95% level of confidence as p-value<0.05. Thus,  $V^*$  is principal in single process parameters setting which should be paid more attention in DIW for the selected ink.

Source	DOF	Sum of squares (SS)	Mean squares (MS)	F-ratio	p value	Contribution (%)
V <sub>n</sub>	2	62.90	31.45	1.21	0.349	6.37
$V^*$	2	274.31	137.15	5.26	0.035	27.78
$H^{*}$	2	65.58	32.79	1.26	0.335	6.64
$v_n \times V^*$	4	263.16	65.79	2.52	0.124	26.65
$v_n \times H^*$	4	69.26	17.31	0.66	0.635	7.01
$V^* \times H^*$	4	43.52	10.88	0.42	0.792	4.41
Error	8	208.77	26.10			21.14
Total	26	987.50				100

Table 3.5 Mean SNR response table for dimensional error of main experiments in step 1

## 3.4.2 Optimization of printed rectangular objects

#### (1) Line width under optimal process parameters

At the beginning of step 2, lines are printed using optimal process parameters obtained in step 1 to get line width under optimum condition. Average width of the optimal printed line is calculated using Eq. (3.5) as 1.31 mm.

#### (2) Single-factor tests

In order to get a layer from lines, distance between lines  $d_i$  is calculated by Eq. (3.4). In Eq. (3.4), average width of optimal lines  $\bar{w}_o$  is obtained at the beginning of step 2; and only single-factor  $R_w$  determines printing results in step 2. Single-factor tests, containing 5

experimental runs, are conducted as shown in Table 3.6 to find the optimal value of  $R_w$ . The lower-the-better SNR is used and results are listed in Table 3.6. Higher SNR represents better dimensional accuracy. Therefore, optimal  $R_w$  is found as:  $R_w = 0.9$ .

Experiment number	NR1	NR2	NR3	NR4	NR5
$R_{_W}$	0.5	0.6	0.7	0.8	0.9
SNR of dimensional error	1.96	0.88	1.73	0.38	16.95

Table 3.6 Single-factor tests for step 2

Consequently, optimal DIW process parameters for a layer fabricated in the prepared ink are selected as:  $v_n = 5 \text{ mm/s}$ ,  $V^* = 0.8$ ,  $H^* = 0.9$ ,  $R_w = 0.9$ .

## **3.5 Experimental verifications**

To verify the selected process parameters and the parameters robustness on other shapes and other materials; parameter adaptability in 3D parts printing from printed layers' analyses for the proposed method and parameter adaptability in constructs fabricated as 100% infill or with porosities. Experimental verifications are presented in this section.

#### (1) Experimental verification for method robustness on shapes

To validate that the optimum conditions can be generalized to layers in other shapes, three shapes as Shape A (disk), Shape B (leaf) and Shape C (maple leaf) are printed under optimal condition achieved by proposed method and condition A ( $v_n = 8 \text{ mm/s}$ ,  $V^* = 1$ ,  $H^* = 0.9$ ,  $R_w = 0.8$ ). As shown in Figure 3.7 (a), the dimensional quality under optimal condition is higher than that under condition A, verifying the method robustness in other shapes.

#### (2) Experimental verification for method robustness on materials

To verify the method robustness on materials, a well-printable cellulose-based ink is chosen proposed by the literature [68]. The ingredients of the cellulose-based ink are: 2.36% cellulose fibers, 0.59% hydroxyethylcellulose (HEC), 1.77% carboxymethyl cellulose (CMC), 0.47% montmorillonite, 0.47% citric acid (CA) and 94.34% demineralized water. The viscosity of cellulose-based ink ( $\mu_0 = 1650 \ Pa \cdot s$ ;  $\tau_0 = 90 \ Pa$ ;  $K = 133 \ Pa \cdot s^n$ ; n = 0.268) is much lower than that of Nivea Crème ( $\mu_0 = 1.58 \times 10^6 \ Pa \cdot s$ ;  $\tau_0 = 563 \ Pa$ ;  $K = 867 \ Pa \cdot s^n$ ; n = 0.045). Thus, the cellulose-based ink has no shape retention ability after extrusion, which is just able to be printed in one layer.

The optimized process parameters for the cellulose-based ink in DIW obtained using the proposed method are:  $v_n = 10 \text{ mm/s}$ ,  $V^* = 0.6$ ,  $H^* = 0.3$ ,  $R_w = 0.5$ . As shown in Figure 3.7 (a),

printed layers in three shapes using the cellulose-based ink have high dimensional accuracy same as Nivea Cràme, verifying the method robustness on materials. Moreover, compared with the optimized process parameters for cellulose-based ink (low viscosity) and Nivea Cràme (high viscosity), it could be concluded that ink with higher viscosity in DIW needs smaller values for  $v_n$  and larger values for  $v^*$ ,  $H^*$  and  $R_w$ .

#### (3) Experimental verification for parameter adaptability in 3D parts printing

In order to verify the adaptability of optimized process parameter from printed layers' analyses in 3D parts printing, three 3D models are printed using the same optimized process parameters and layer height is set as h for printed layers in Nivea Cr àme based DIW. As shown in Figure 3.7 (b), the printed 3D parts had good dimensional quality by comparing printed parts under optimal condition and condition A ( $v_n = 8$  mm/s,  $v^* = 1$ ,  $H^* = 0.9$ ,  $R_w = 0.8$ ), verifying that the proposed method has parameter adaptability in 3D parts printing from printed layers.

# (4) Experimental verification for parameter adaptability in constructs with porosities

To verify the adaptability of optimized process parameter for constructs with porosities, confirmation tests are conducted as shown in Figure 3.8. Two grids named as Grids A and Grids B are designed as shown in Figure 3.8 (a): the total dimensions of grids A and grids B are same in 31.2 mm × 31.2 mm; and the dimensions of porosity in grids A and grids B are 3 mm × 3 mm and 6.8 mm × 6.8 mm, respectively. As shown in Figure 3.8 (b) and Figure 3.8 (c), the printed single-layer and 10-layers grids had good dimensional quality by comparing printed grids under optimal condition and condition A ( $v_n = 8$  mm/s,  $V^* = 1$ ,  $H^* = 0.9$ ,  $R_w = 0.8$ ), verifying that the proposed method has parameter adaptability in constructs with porosities.



Figure 3.7 Experimental verifications for the selected process parameters in (a) verification of method robustness on layer shapes and materials; (b) verification for parameter adaptability in 3D parts printing



Figure 3.8 Experimental verifications for the selected process parameter in constructs with porosities: (a) two designed grids: grids A and grids B; (b) printed grids A under optimal condition and condition A in single layer and 10-layers; (c) printed grids B under optimal condition and condition A in single layer and 10-layers.

## **3.6** Conclusion

In this chapter, ink material properties are characterized and optimal process parameters setting is selected to provide the basis for modeling inputs. For ink material properties characterization, density, surface tension, static contact angle and rheology properties are obtained for the used ink.

For process parameters selection, the DIW process parameters are identified through process analyses and a two-step method is proposed to optimize DIW process parameters for dimensional accuracy and analyze the significance of each process parameter.

In the DIW process parameters identification, DIW process parameters for printed layers are divided into two categories and identified by process analysis as: 1) process parameters for printing a line and 2) extra process parameter from lines to a layer. The process parameters identification considers the relationship between intermediate process parameters as well as main sources of errors in the experiments. Thus, the process parameters selection method improves the efficiency and accuracy of the optimization process. In the two-step optimization method for identified DIW process parameters, Step 1 is to optimize process parameters for printing a line and Step 2 is to optimize the parameter from lines to a layer. Experimental verifications verify the proposed method and the its robustness on other shapes and other materials; parameter adaptability in 3D parts printing from printed layers' analyses for the

proposed method and parameter adaptability in constructs fabricated as 100% infill or with porosities. This proposed two-step optimization method satisfies the requirement of high quality DIW process by finding optimum process parameters setting with minimum materials and time. The proposed process parameters selection method allows a rapid and reproducible process parameters optimization of a wide variety of inks in DIW.

In conclusion, ink material property characterization and process parameters selection are conducted and presented in this chapter in order toprovide the basis for the numerical modeling of DIW.

## Chapter 4: Numerical modeling, experimental verification and process analysis for DIW

## **4.1 Introduction**

As summarized in the literature in Section 2.3.1, outputs of modeling for DIW include freeform extruded filament (FEF), deposited filament (DF), deposited corner, printed layer and 3D part. This thesis focuses on the numerical simulations of the most basic elements in DIW: FEF, DF and deposited corner.

Firstly, volume of fluid (VOF) method is selected as numerical simulation method and introduced. Then, numerical simulations, experimental verifications and process analyses for DIW are presented.

For numerical simulation of FEF, there is few works on modeling and evaluation of FEF based on numerical simulation methods for DIW. Numerical simulation modeling of FEF should fully consider ink's properties and process parameters as the quality of FEF depends both on ink's material properties and process parameters setting [119]. Evaluation of FEF should consider both the mean diameter and the stability as these two indicators have the most significant influence on the printing quality [174]. The aim of process modeling and analysis of FEF based on numerical simulations is to establish a model of FEF with numerical simulation method and then evaluate the FEF based on this model. First, model of FEF is established using numerical simulation method and two evaluation indicators, mean diameter and stability, are proposed to evaluate the FEF. Then, the selected ink, Nivea Cràme, is used under three levels of piston velocity to verify the numerical simulation. After experimental verification, the model and evaluation indicators are used to analyze effect of the piston velocity on FEF and find suitable printable windows for process parameters.

For numerical simulation of DF, several researchers have established numerical prediction models for DF in MEAM. Comminal et al. [150] established a numerical model of deposited filaments in MEAM but this work lacked experimental validation. Serdeczny et al. [175] used an experimental procedure to validate the numerical model and investigated the influence of the processing conditions on cross-section of a strand printed by material extrusion AM through a numerical model. Göhl et al. [147] used a computational fluid dynamics (CFD) simulation

tool to study the effect of printing parameters on deposited filaments in bio-printing. Gosset et al. [176] presented a numerical study of the deposition of a single strand of poly-lactic acid (PLA) by MEAM via a CFD model. Although the previous works found that DF is significantly influenced by process parameters, they often failed to realize full quantitative characterizations of the detailed influence of the process parameters on the deposition status and profile dimension of deposited filaments. Meanwhile, there is few works on numerical prediction for deposited filaments in DIW by fully considering the ink material properties and process parameters setting. Thus, it is crucial and desirable to fully study and predict the deposition status and profile dimension of the deposited filaments in DIW processes based on numerical prediction.

In this chapter, an improved 3D numerical prediction model of deposited filaments in DIW is established with VOF method to predict deposition status and profile dimension of deposited filaments. Filaments deposition experiments are conducted using the selected ink to verify the proposed model. Using the proposed numerical model, the deposition status is divided into three statuses and profile dimension under each status is predicted. The effect of process parameters including the dimensionless nozzle velocity and the dimensionless height on deposition status and profile dimension has been quantified using numerical simulations for the first time. The numerical simulation of DF demonstrates a material-saving and effective approach for prediction of deposition status and profile dimension is been profile dimension of the DF and the investigation of the effects of process parameters in DIW with computer based numerical simulations.

For numerical simulation of deposited corner, to fully understand the DIW process and improve the geometrical quality of parts in DIW, numerical simulation methods have been widely used to model the MEAM process [147, 150, 152, 177]. With the benefits of the proposed numerical simulations, researchers have successfully evaluated the printability of new prepared inks, found the optimized process parameters, analyzed the material extrusion process and realized digital twin of the MEAM process with small consumption of material and experimental time [178-180]. Comminal et al. simulated the strand deposition [150] and the material deposition along a toolpath with a sharp corner [152] with computational fluid dynamics (CFD) models to study the effect of process parameters on deposited filaments and corners, respectively. G öhl et al. [147] conducted computer based simulations for DIW to evaluate newly developed inks. Tu et al. [177] established a model of freeform extruded filaments with numerical simulation and then evaluate the filaments based on the model for

DIW. However, the previous work [152] for numerical simulation of deposited corners could only achieve the corner simulation under the condition of small angle which is less than 90  $^{\circ}$  but failed to realize corner simulation of any angle. Thus, to overcome the limitation of the previous research for numerical simulation of deposited corners and fully realize DIW process modeling based on the application of numerical simulation, it is crucial and required to propose an improved numerical simulation to model deposited corners of any angle.

In this chapter, 3D numerical simulations of deposited corners of any angle in DIW are established with VOF method and corner deposition experiments are conducted using the selected ink to validate the proposed numerical simulation. The numerical simulation of deposition corner overcomes the limitation of previous research works in numerical simulation of deposited corners and demonstrates an effective approach for prediction of deposited corns of any angle in DIW with computer based numerical simulation.

## 4.2 Volume of fluid (VOF) method

The 3D numerical modeling for outputs in DIW is a two-phase flow simulation to capture the interface between the ink and air. Numerical methods for two-phase flow problem include level set method [155], phase field method [156], lattice-Boltzmann method [157], direct interface tracking method [158] and VOF method [154]. Among these numerical methods, the VOF method has been widely used in numerical simulation of filaments in MEAM due to its simplicity, robustness and straightforward implementation [159]. Thus, VOF method is adopted as simulation method in this thesis.

#### 4.2.1 Theory of VOF

In VOF, the ink and air are treated as a single continuum and the phase fraction  $\alpha$  is defined to distinguish the interface between the two-phase fluid as follows [181]:

$$\alpha = \frac{V_i}{V_m} \tag{4.1}$$

Where  $\alpha$  is the phase fraction for a mesh;  $V_i$  is the volume of the ink in a mesh;  $V_m$  is the total volume of a mesh. As shown in Figure 4.1,  $\alpha = 0$  when the mesh is filled with air and  $\alpha = 1$  when the mesh is filled with ink. In the meshes along boundary between ink and air, the value of  $\alpha$  belongs to (0,1).  $\alpha = 0.5$  is defined as the cut-off value to capture the sharp front of interface between the ink and air.


Figure 4.1 Illustration of phase fraction in volume of fluid (VOF) method

Fluid properties of the single continuum are weighted with the phase fraction as follows:

$$\rho_s = \alpha \rho + (1 - \alpha) \rho_a \tag{4.2}$$

$$\mu_s = \alpha \mu + (1 - \alpha) \mu_a \tag{4.3}$$

Where  $\rho_s$  and  $\mu_s$  is density and viscosity of the single continuum;  $\rho$  and  $\rho_a$  is density of the ink and air, respectively;  $\mu$  and  $\mu_a$  is viscosity of the ink and air, respectively.  $\mu$  is expressed using the Hershel-Bulkley model (HBM) due to its shear-thinning behaviour as shown in Eq. (3.2).

The following assumptions about the numerical simulations of DIW are formulated:

- The deposition process is considered isothermal as the process is conducted at room temperature;
- The material is considered incompressible with constant  $\rho$ ;
- The ink adheres to the surfaces of the nozzle without slip and the static contact angle between ink and the substrate is considered;
- The filaments flow is laminar.

Based on these assumptions, the governing equations for the numerical simulation include continuity equation, momentum equilibrium equation and phase fraction equation. Each equation is written as follows [182].

Continuity equation:

$$\nabla \cdot \mathbf{U} = 0 \tag{4.4}$$

Where U is velocity field of the fluid.

Momentum equilibrium equation:

$$\frac{\partial \rho_s \mathbf{U}}{\partial t} + \nabla \cdot (\rho_s \mathbf{U} \mathbf{U}) = -\nabla p + \nabla \cdot (\rho_s \mu_s \nabla \mathbf{U}) + \rho_s \mathbf{g} + \mathbf{F}_{\sigma}$$
(4.5)

Where *p* is the pressure in the fluid; **g** is the gravitational acceleration vector;  $\mathbf{F}_{\sigma}$  is surface tension.  $\mathbf{F}_{\sigma}$  is calculated as follows:

$$\mathbf{F}_{\sigma} = \sigma \kappa \nabla \alpha \tag{4.6}$$

where  $\sigma$  is the surface tension coefficient;  $\kappa$  is the surface curvature which is depended on the shape of deposited ink on the substrate.  $\kappa$  is computed from local gradients in the surface normal to the interface as follows [183]:

$$\kappa = \frac{1}{|\mathbf{n}|} \left( \left( \frac{\mathbf{n}}{|\mathbf{n}|} \cdot \nabla \right) |\mathbf{n}| - \nabla \cdot \mathbf{n} \right)$$
(4.7)

where  $\mathbf{n} = \nabla \alpha$  is the normal vector to the ink surface. Wall adhesion between deposited ink and substrate is considered in the model based on the use of the static contact angle as:

$$\hat{\mathbf{n}} = \hat{\mathbf{n}}_{w} \cos \theta_{c} + \hat{\mathbf{t}}_{w} \sin \theta_{c} \tag{4.8}$$

where  $\hat{\mathbf{n}} = \mathbf{n} / |\mathbf{n}|$  is the unit vector normal to the ink surface,  $\hat{\mathbf{n}}_{w}$  and  $\hat{\mathbf{t}}_{w}$  represents the unit vector normal and tangent to the substrate, respectively,  $\theta_{c}$  is the static contact angle between the ink and substrate.

Phase fraction equation:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{U}) + \nabla \cdot (\alpha (1 - \alpha) \mathbf{U}_{r}) = 0$$
(4.9)

Where  $U_r$  is velocity vector compressing two-phase free surface, which represents the velocity difference between two-phase fluids and can be calculated as follows:

$$\mathbf{U}_{\mathbf{r}} = \min(c|\mathbf{U}|, \max|\mathbf{U}|) \frac{\nabla\alpha}{|\nabla\alpha|}$$
(4.10)

Where *c* is controllable compression factor and it is selected as c=1 in the numerical simulation.

## 4.2.2 Implementation of VOF

The free and open-source CFD software OpenFOAM v1912 [184] is used to realize the numerical simulation of the DIW. In the numerical simulation, OpenFOAM v1912 is used to build geometrical model, generate meshes, determine boundary conditions and solve governing equations. Especially, the governing equations in VOF are solved based on the solver for two incompressible, isothermal immiscible fluids using VOF method with optional mesh motion and mesh topology changes including adaptive re-meshing, *interFoam*. PIMPLE algorithm, a combined algorithm of the pressure-implicit split-operator (PISO) and the semi-implicit method for pressure-linked equations (SIMPLE) algorithms, is chosen as the numerical algorithm for *interFoam* solver.

After numerical simulation in OpenFOAM v1912, ParaView, which is an open-source, multi-platform data analysis and visualization application [185], is used to build visualizations and analyze simulation data.

In this thesis, hardware condition for the numerical simulations is as follows:

Computer: Dell precision T1700; processor in computer: Intel XEON; simulation software: OpenFOAM v1912.

#### **4.3 Numerical simulation of FEF**

### 4.3.1 Numerical Modeling

As shown in Figure 4.2 (a), FEF is produced by extruding ink in the syringe through the nozzle into the air with the piston movement. Dimensions of the geometrical model of FEF in DIW include: the piston diameter  $D_p$ ; the initial filled length of ink  $L_0$ ; the nozzle inner diameter  $d_n$ ; the nozzle outer diameter  $D_n$ ; the nozzle length  $L_n$ ; the gap between nozzle bottom and substrate h. In this modeling, h is set as 26 mm to avoid FEF touching the substrate.  $D_p$ ,  $d_n$ ,  $D_n$ ,  $L_n$  and  $L_0$  are set to match the actual device dimensions: 21.6 mm, 0.84 mm, 1.22mm, 18 mm, 30 mm, respectively. Figure 4.2 (b) presents the 3D model established in OpenFOAM for FEF at the initial time, where red regime represents the ink and blue regime represents the air. As shown in Figure 4.2 (c), the 3D model is simplified into a 2D axisymmetric model by capturing 1/120 of the 3D model in the circumferential direction to reduce computation cost under the axisymmetric laminar flow condition for the ink extrusion.



Figure 4.2 Geometrical model of FEF in numerical simulation for DIW: (a) dimensions of the geometrical model; (b) established 3D model at the initial time; (c) simplified 2D axisymmetric model at the initial time

OpenFOAM is designed as a code for 3D space and defines all meshes as 3D meshes, but wedge type meshes are used for 2D axisymmetric problems specifically [186]. Thus, wedge type meshes are used for the simplified 2D axisymmetric model as shown in Figure 4.3 (a), where lengths and widths of meshes in the same area are set nearly same and meshes in the junction of different areas are refined to improve calculation accuracy. Total number of the meshes is 18996. Boundary conditions are grouped into 5 categories and are defined as shown in Figure 4.3 (b) and Table 4.1.



Figure 4.3 Meshes and boundary conditions for model of FEF in numerical simulation for DIW: (a) meshes; (b) boundary conditions

Table 4.1 Definition of	of boundary conditions	for numerical	model of FEF
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Name	Physical meaning	Туре	Setting
B1	Piston	Moving boundary	Velocity is equal to piston velocity
B2	Inner walls of syringe; walls of nozzle and substrate	No-slip boundary	No-slip
B3	Air	InletOutlet boundary	Depended on dynamic calculation
B4	Symmetrical axis	Symmetrical boundary	Empty condition
В5	Front and back side symmetrical sections	Wedge boundary	Symmetrical condition

## 4.3.2 Experimental verification

In order to validate the proposed numerical model of FEF, the selected ink Nivea Crème is used as ink for FEF extrusion tests in a DIW 3D printer. As shown in Figure 4.4 (a), a piston driven DIW 3D printer TM-081 (Tobeca Company, France) is used to extrude ink in the syringe into FEF in the air; and a camera (Canon LEGRIA HF R86 Noir, Canon Inc., Japan) is used to take photos of FEF. As shown in Figure 4.4 (b), the extrusion tool in the DIW 3D printer is composed of a 30mL syringe (Braun Melsungen AG, Germany) and a precision engineered fluid dispensing nozzle (Nordson EFD, USA). Dimensions of extrusion tool are: h = 26 mm,  $D_p = 21.6$  mm,  $d_n = 0.84$  mm,  $D_n = 1.22$ mm,  $L_n = 18$  mm,  $L_0 = 30$  mm (same as the setting in numerical simulation modelling in Section 4.3.1). The ink material properties of Nivea Crème are used the value in Table 3.1 obtained in Section 3.2.3.



Figure 4.4 Experimental validation setup for the numerical simulation of FEF: (a) producing FEF using DIW 3D printer and observing FEF using camera; (b) extrusion tool in the DIW 3D printer

Disregarding ink compressibility, the mass conservation for the FEF producing process is expressed as:

$$v_p / v_e = (d_n / D_p)^2$$
 (4.11)

Where  $v_p$  is the piston velocity,  $v_e$  is average velocity of FEF.

To verify the numerical simulation of FEF considering the universality for different process parameters, 3 levels of  $v_p$  are set by setting  $v_e$  from 5 mm/s to 15 mm/s at fixed intervals of 5 mm/s, which are on the printable range. The 3 levels setting for  $v_p$  is summarized in Table 4.2. The simulation calculation time of FEF is 10 minutes.

Table 4.2 Piston velocity setting in the experimental validation for numerical simulation of FEF

Levels	$v_1$	v <sub>2</sub>	v <sub>3</sub>
$v_e$ (mm/s)	5	10	15
$v_p \ (10^{-3} \text{ mm/s})$	7.56	15.12	22.68

Simulation and experimental results for the selected ink Nivea Crème under 3 levels of  $v_p$  are plotted in Figure 4.5. Here, all images are plotted using the same graphical scale in order to provide a direct comparison of simulation and experimental results. Modeling is verified by comparing simulation and experimental results for shape and diameter accuracy. For shape, all simulation results had continuous extruded profiles in accordance with experimental results by observing images in Figure 4.5. Diameter prediction accuracy is defined as verification indicator to verify the prediction accuracy of the model as follow:

$$E_{f} = \sqrt{\frac{\sum_{i=1}^{N_{f}} e_{fi}^{2}}{N_{f}}}$$
(4.12)

Where  $E_f$  is diameter prediction accuracy of numerical simulation of FEF,  $N_f$  is the number of measurement points in FEF where  $N_f$  points are evenly set on the FEF starting from the nozzle bottom,  $e_{fi}$  is the diameter difference between experimental and simulation results at *i* point.

In this verification, the length of FEF is 5.2 mm; the interval of measurement points is 0.5 mm and  $N_f$  is 10. Diameter prediction accuracy for the Nivea Cr ème are 0.02 mm, 0.08 mm and 0.04 mm for  $v_1$ ,  $v_2$  and  $v_3$ , respectively, where the maximum error is 0.08 mm and the maximum relative error is 9.52%, verified the numerical simulation model of FEF had a high diameter accuracy. Thus, the model is verified both from shape and diameter accuracy.



Figure 4.5 Simulation and experimental results of FEF under 3 levels of piston velocities for the selected ink Nivea Crème

# 4.3.3 Process analysis

After experimental verification, the simulation model of FEF is used to evaluate the effect of the piston velocity on the FEF and find suitable printable windows for process parameters by defining evaluation indicators of FEF.

## (1) Evaluation indicators

Defined evaluation indicators of FEF include mean diameter and stability as continuous and tubular FEF with diameters close to the actual nozzle inner diameter is the basic requirement for a successful extrusion-based AM [187].  $N_f$  measuring points are set along the FEF uniformly from nozzle bottom at fixed sampling intervals of 0.5 mm and diameter on each

measuring point is measured as  $d_{fi}(i=1,2,...,N_f)$ . Mean diameter and stability of FEF are expressed using average and standard deviation of  $d_{fi}(i=1,2,...,N_f)$ , respectively.

#### (2) Evaluation of FEF

Based on the evaluation indicators, process analysis is conducted. Firstly,  $v_p$  are set by setting  $v_e$  from 1 mm/s to 20 mm/s with Eq. (4.11) and used as input conditions in the proposed numerical model of FEF. Then, the two evaluation indicators are used to evaluate FEF under different piston velocities based on the model. As shown in Figure 4.6, there is no continuous and stable FEF when setting of  $v_e$  is lower than 2 mm/s for the Nivea Cr ème as piston velocity should be large enough to let FEF overcome yield stress and surface tension to produce continuous and stable filaments. The minimum setting of  $v_e$  to produce stable FEF for the ink depends on yield stress and surface tension coefficient of the ink.

When setting of  $v_e$  is higher than minimum setting of  $v_e$  to produce stable FEF, mean diameters of FEF decrease with increasing setting of  $v_e$  for the Nivea Cr àme. Especially, mean diameters of FEF get closer to the nozzle inner diameter as setting of  $v_e$  increases ranging from 1 mm/s to 10 mm/s and is equal to nozzle inner diameter when setting of  $v_e$  is 10 mm/s (Figure 4.6 (a)). Then, it moves further away from the nozzle inner diameter as the setting of  $v_e$  is higher than 10 mm/s. As shown in Figure 4.6 (b), stability decreases firstly and then increases as setting of  $v_e$  increases ranging from 1 mm/s to 20 mm/s for the Nivea Cr àme. Considering the requirement that FEF should have mean diameter close to nozzle inner diameter and good stability, printable window of setting of  $v_e$  for FEF is summarized from Figure 4.6: 5 mm/s-15 mm/s for Nivea Cr àme. This is consistent with the optimal  $v_e$  (5 mm/s) obtained by the experimental method in Section 3.3.



Figure 4.6 Evaluation of the FEF for the Nivea Crène using the defined two evaluation indicators as: (a) mean diameter; (b) stability

# 4.4 Numerical simulation of DF

## 4.4.1 Numerical Modeling

Numerical modeling for the 3D profile of DF is established based on the use of free and open-source CFD software OpenFOAM v1912 as shown in Figure 4.7. Because the ink extrusion and deposition process are considered as an isothermal, incompressible and laminar flow, the average velocity on each cross section in the nozzle is the same and it can be expressed as Eq. (4.11) based on conservation of mass.

According to Eq. (4.11), the flow situation in syringe has no effect on  $v_e$ . Thus, the 3D geometrical model is simplified as a combination of the nozzle, substrate and air by neglecting the syringe to improve computational efficiency as shown in Figure 4.7 (a). As presented in Figure 4.7 (b), the critical parameters in the model include the inner diameter of nozzle  $d_n$ , the outer diameter of nozzle  $D_n$ , the average velocity of ink in nozzle  $v_e$ , the nozzle length  $L_n$ , the distance between nozzle bottom and substrate h, and the nozzle velocity  $v_n$ . In the numerical simulation of DF, the values of  $d_n$  and  $D_n$  are set as 0.84 mm and 1.22 mm, which match the actual dimensions of DIW 3D printer in experimental verification, respectively.  $v_e$  is calculated using Eq. (4.11) where the value of  $D_p$  is set as 21.6 mm. As the nozzle length has no effect on  $v_e$  and the final DF, the value of  $L_n$  is set as 2.44 mm which is smaller than practice nozzle length (18 mm) to reduce computational time. To avoid the model becoming a complex dynamic-mesh model which needs a large amount of computational time, the position of nozzle is fixed while the substrate is attached with a moving velocity  $v_n$  in the boundary setting as the

movements of the nozzle and substrate are relative to each other. As shown in Figure 4.7 (c), meshes are refined in the region of DF to improve calculation efficiency and accuracy.

The initial condition of phase fraction is shown in Figure 4.7 (d) where red region represents the ink and blue region represents the air, meaning that the ink is filled in the nozzle at the initial time. Finally, the 3D profile of DF is obtained through VOF by capturing the sharp front of interface where the value of  $\alpha$  is 0.5. And the visualization of the deposited filaments is realized using the open-source, multi-platform data analysis and visualization software, ParaView.



Figure 4.7 Numerical modeling of 3D profile of DF: (a) 3D geometrical model; (b) critical parameters in the model; (c) generated meshes; (d) initial condition of phase fraction

## 4.4.2 Experimental verification

Yuk and Zhao [188], Comminal et al. [150] and Athanasiadis et al. [125] have summarized that the deposition and the profile dimension of the DF in MEAM are significantly influenced by the dimensionless nozzle velocity  $V^* = v_n / v_e$  (ratio of nozzle velocity  $v_n$  to average velocity of ink in the nozzle  $v_e$ ) and the dimensionless height  $H^* = h/d_n$  (ratio of distance between nozzle bottom and substrate *h* to inner diameter of nozzle  $d_n$ ).

The deposition process and the process parameters of DIW are illustrated in Figure 4.8 (a). Ink is filled in the syringe at the initial filled length and the full nozzle first. When piston started moving at a fixed velocity  $v_p$ , ink is extruded out from nozzle. By setting the distance between nozzle bottom and substrate as h and the nozzle velocity related to substrate in the horizontal direction as  $v_n$ , the FEF is deposited on the substrate. Through observations of crosssectional shapes under different process parameters, it is summarized that there are three deposition statuses for cross-sectional shapes of DF: over-deposition, pressed-deposition and freeform-deposition. When h is much smaller than  $d_n$  or  $v_n$  is much smaller than  $v_e$ , the DF is in over-deposition status. In over-deposition status as shown in Figure 4.8 (b), excessive ink is squeezed out beyond the outer diameter of the nozzle and width, height of DF are irregular and cannot be predicted. When h and  $v_n$  increased, the status would change to pressed-deposition as shown in Figure 4.8 (c) first and then change to freeform-deposition as shown in Figure 4.8 (d). In pressed-deposition status, the height of DF  $h_d$  is equal to h as DF is pressed by nozzle bottom and the two ends of the cross-sectional of DF are regular semicircles with a diameter of  $h_d$ . In freeform-deposition status, the filament is deposited without nozzle contact and crosssectional shape is a part of circle dependent on the static contact angle  $\theta_c$  between the ink and the substrate. The simulation calculation time of DF is 40 minutes.

To determine deposition statuses, the dimensionless nozzle velocity  $V^*$  and the dimensionless height  $H^*$  are used. Using the law of conservation of mass, the conditions of over-deposition and freeform-deposition could be expressed as Eq. (4.13) and Eq. (4.14), respectively.

$$\frac{\pi}{4}d_n^2 v_e \ge h \cdot D_n \cdot v_n \tag{4.13}$$

$$\frac{\pi}{4}d_n^2 v_e \le \left(\theta_c - \frac{\sin 2\theta_c}{2}\right) \left(\frac{h}{1 - \cos \theta_c}\right)^2 v_n \tag{4.14}$$

Then, Eq. (4.13) and Eq. (4.14) are simplified as Eq. (4.15) and Eq. (4.16), respectively using  $V^*$  and  $H^*$ .

$$V^* \le \frac{\pi}{4\beta} \cdot \frac{1}{H^*} \tag{4.15}$$

where  $\beta$  is the ratio of  $D_n$  to  $d_n$  ( $\beta = D_n / d_n$ ).

$$V^* \ge \frac{\pi}{4\gamma} \cdot \left(\frac{1}{H^*}\right)^2 \tag{4.16}$$

where  $\gamma$  represented  $\left(\theta_{c} - \frac{\sin 2\theta_{c}}{2}\right) \left(\frac{1}{1 - \cos \theta_{c}}\right)^{2}$ .

The dividing line 1 (solid red line) and dividing line 2 (solid blue line) described by Eq. (4.15) and Eq. (4.16) are plotted in Figure 4.8 (d) to predict deposition statuses under different  $V^*$  and  $H^*$ . Combinations of  $V^*$  and  $H^*$  are divided into three areas by dividing line 1 and dividing line 2: area below dividing line 1 represents over-deposition; area between dividing line 1 and dividing line 2 represents pressed-deposition and area above dividing line 2 represents freeform-deposition.



Figure 4.8 Analyses of deposition statuses and cross-sectional shapes of DF: (a) illustration of deposition process and process parameters; three deposition statuses for cross-sectional shapes of DF as (b) over-deposition, (c) pressed-deposition and (d) freeform-deposition; (e) cross-sectional shapes statuses division

Thus, to fully verify the numerical simulation of DF in deposition status, width and height. First,  $v_e$  is set as two-level process parameter which is 6 mm/s and 9 mm/s to investigate the influence of  $v_e$  on the deposition status. Then, at each level of  $v_e$ ,  $v^*$  is varied from 0.4 to 1.2 at a fixed interval of 0.4 and  $H^*$  is varied from 0.3 to 1.5 at a fixed interval of 0.3 to investigate the influence of  $v^*$  and  $H^*$  on deposition status.

The quantitative comparison of the profile dimension is conducted by measuring width and height of the cross-section of the DF. A piston-driven DIW 3D printer TM-081 (Tobeca Company, France) with the selected ink is used to conduct filaments deposition experiments (Figure 4.9). In the experiments, process parameters are set first and then three 80 mm long filaments are deposited on a glass substrate and a camera (Canon LEGRIA HF R86 Noir, Canon Inc., Japan) is used to capture top and side views of deposited filaments to determine the deposition status and profile dimension of deposited filaments. The width of deposited filaments is measured at a fixed sampling interval of 5 mm for three filaments in the top view and the height is measured in the end face for three filaments in the side view. The average and standard deviation are calculated for 45 sampling points in width measurement and 3 sampling points in height measurement. Experimental width and height are expressed as the mean  $\pm$ standard deviation.



Figure 4.9 Experimental setup for filaments deposition experiments and corners deposition experiments

#### 4.4.2.1 Experimental verification of deposition status for DF

Figure 4.10 represents the characterization of the three deposition statuses in experimental results from top view and side view and the characterization of the three deposition statuses in simulated results from 3D shape and cross-section, which show a good consistency of experimental and simulated results in the deposition status characterization. In the over-deposition status, the two ends of the cross-section are irregular shapes which are higher than h. In the pressed-deposition status, the height of cross-section is equal to h and the two ends of the as-deposited filaments possess semicircle shapes with a diameter of the same value of h. In the freeform-deposition, the cross-section nearly takes a circle shape.



Figure 4.10 Characterization of deposition status in experimental and simulated results: (a) over-deposition; (b) pressed-deposition; (c) freeform-deposition

In order to investigate the influence of the process parameters on the deposition status, the experimental and simulated deposition status under different process parameters are compared. By using the symbols +,  $\blacksquare$  and  $\bullet$  to represent over-deposition, pressed-deposition and freeform-deposition respectively, the experimental statuses of the deposited filaments under different process parameters are summarized in Figure 4.11. Correspondingly, the simulated deposited filaments under different process parameters are plotted in Figure 4.12 by using pink, green and cyan backgrounds to represent over-deposition, pressed-deposition and freeform-deposition respectively. It can be found that the effectiveness of the numerical prediction for the deposited filaments is validated as the simulated deposited statues dividing results are consistent with the experimental results and is also consistent with the idealized results.



Figure 4.11 Experimental deposited status of the deposited filaments under different process parameters: (a) the value of  $v_e$  is set as 6 mm/s; (b) the value of  $v_e$  is set as 9 mm/s



Figure 4.12 Simulated deposition status of the DF under different process parameters: (a) the value of  $v_e$  is set as 6 mm/s; (b) the value of  $v_e$  is set as 9 mm/s

#### 4.4.2.2 Experimental verification of profile dimension for DF

The DF in pressed-deposition and freeform-deposition have regular width and height and can finally be deposited for 3D parts with high quality but over-deposition with irregular profile leading to inferior quality should be avoided. Thus, prediction for width and height in pressed-deposition and freeform-deposition is meaningful for DIW quality evaluation and control. To verify the prediction accuracy of profile dimension for the proposed numerical model, experimental results of width and height under different process parameters setting are measured and listed in Table 4.3 and Table 4.4 where the symbol + represented over-deposition status. Correspondingly, the simulated width and height are listed in Table 4.5 and

Table 4.6. The relative errors between experimental and the simulated width and height are calculated using the data from Table 4.3 to

Table 4.6 and listed in Table 4.7 and Table 4.8.

Table 4.3 Experimental width under different process parameters (width unit: mm)

$H^*$	0.	.3	0	.6	0	.9	1	.2	1.5		
V*	Ve/(n	nm/s)	V <sub>e</sub> /(n	nm/s)	V <sub>e</sub> /(mm/s)		Ve/(n	nm/s)	Ve/(mm/s)		
·	6	9	6	9	6	9	6	9	6	9	
1.2	+	+	1.00±0.04	1.07±0.06	0.81±0.03	0.79±0.03	0.80±0.05	0.77±0.03	0.79±0.03	0.77±0.03	
0.8	+	+	+	+	1.10±0.02	1.06±0.04	0.97±0.03	0.95±0.04	0.97±0.03	0.95±0.03	
0.4	+	+	+	+	+	+	+	+	1.43±0.05	1.35±0.04	

$H^*$	0	.3	0	0.6 0.9 1		.2	1.5				
V*	Ve/(n	nm/s)	V <sub>e</sub> /(r	nm/s)	V <sub>e</sub> /(mm/s)		Ve/(n	nm/s)	Ve/(mm/s)		
•	6	9	6	9	6	9	6	9	6	9	
1.2	+	+	0.5±0.01	0.5±0.02	0.75±0.01	0.75±0.01	0.80±0.05	0.77±0.01	0.79±0.03	0.77±0.01	
0.8	+	+	+	+	0.75±0.01	0.75±0.01	0.97±0.03	0.95±0.04	0.97±0.03	0.95±0.03	
0.4	+	+	+	+	+	+	+	+	1.25±0.02	1.25±0.01	

Table 4.4 Experimental height under different process parameters (height unit: mm)

Table 4.5 Simulated width ur	ender different process par	rameters (width unit: mm)
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$\mathrm{H}^{*}$	0.	0.3 0.6		0.9		1.2		1.5		
$\mathbf{V}^*$	V <sub>e</sub> /(n	nm/s)	V <sub>e</sub> /(n	nm/s)	V <sub>e</sub> /(mm/s)		V <sub>e</sub> /(mm/s)		V <sub>e</sub> /(mm/s)	
• _	6	9	6	9	6	9	6	9	6	9
1.2	+	+	1.00	1.00	0.89	0.87	0.81	0.80	0.81	0.80
0.8	+	+	+	+	1.10	1.10	0.94	0.92	0.97	0.94

0.4 + + + + + + + + + + 1.35 1.30
-----------------------------------

$H^*$	0.	3	0	.6	0	.9	1	.2	1	.5
V*	Ve/(n	nm/s)	V <sub>e</sub> /(n	nm/s)	Ve/(r	nm/s)	V <sub>e</sub> /(r	nm/s)	Ve/(n	nm/s)
• _	6	9	6	9	6	9	6	9	6	9
1.2	+	+	0.50	0.50	0.73	0.71	0.78	0.78	0.78	0.76
0.8	+	+	+	+	0.74	0.74	0.93	0.93	0.90	0.88
0.4	+	+	+	+	+	+	+	+	1.25	1.23

Table 4.6 Simulated height under different process parameters (height unit: mm)

Table 4.7 Relative error of experimental and simulated width under different processparameters

$\mathrm{H}^{*}$	0.	3	(	).6	0	).9	1	.2	1	.5
V*	Ve/(m	nm/s)	Ve/(	mm/s)	Ve/(1	mm/s)	Ve/(r	nm/s)	V <sub>e</sub> /(r	nm/s)
	6	9	6	9	6	9	6	9	6	9
1.2	+	+	0	6.54%	9.88%	10.13%	1.25%	3.90%	2.53%	4.00%
0.8	+	+	+	+	0	3.77%	4.44%	3.16%	0	1.05%
0.4	+	+	+	+	+	+	+	+	5.59%	3.70%

Table 4.8 Relative error of experimental and simulated height under different processparameters

$\mathrm{H}^{*}$	0.	3	0.	6	0	.9	1	.2	1	.5
V*	Ve/(m	nm/s)	Ve/(mm/s)		Ve/(mm/s)		V <sub>e</sub> /(mm/s)		Ve/(mm/s)	
• _	6	9	6	9	6	9	6	9	6	9
1.2	+	+	0	0	2.67%	5.33%	2.50%	1.30%	1.27%	1.30%
0.8	+	+	+	+	1.33%	1.33%	4.12%	2.10%	7.22%	7.37%
0.4	+	+	+	+	+	+	+	+	0	1.60%

The accuracy of the numerical prediction for profile dimension is verified as the maximum relative errors of width and height between the experimental and simulated results are 10.13% and 7.37% respectively, which are significantly improved as compared with the values of 20% and 28% reported in the literature [175]. As shown in Figure 4.13, the numerical perdition accuracy for profile dimension varies with the process parameters setting and the maximum

relative error appears at the edge of the printable window. The maximum relative error of width appears at the edge of the  $v^*$  setting ( $H^* = 0.9$ ,  $v^* = 1.2$ ) and the maximum relative error of height appears at the edge of the  $H^*$  setting ( $H^* = 1.5$ ,  $v^* = 0.8$ ). In these cases, relatively large prediction errors for the profile dimension would generate.



Figure 4.13 Relative error of the experimental and simulated profile dimension under different process parameters for: (a) width when  $v_e$  is set as 6 mm/s; (b) width when  $v_e$  is set as 9 mm/s; (c) height when  $v_e$  is set as 6 mm/s; (d) height when  $v_e$  is set as 9 mm/s

#### 4.4.3 Process analysis

After the experimental validation for the numerical prediction of the deposited filaments, the effects of process parameters on deposited filaments are investigated based on the use of the numerical model. Figure 4.11, Figure 4.12, and Table 4.3 to

Table 4.6 show that the deposition statuses and profile dimension are influenced by  $v^*$ and  $H^*$  while  $v_e$  has no impact when  $v^*$  and  $H^*$  are fixed when  $v_e$  is set in printable window. The reason for this phenomenon is that  $v_n$  and  $v_e$  have the same multiple change when the value of  $v^*$  is fixed  $(v^* = v_n / v_e)$  which causes the effect of changes in  $v_e$  to be offset by the synchronous changes in  $v_n$ .

The combination of  $v^*$  and  $H^*$  influence the deposition status and profile dimension. In order to investigate the effect of  $v^*$  and  $H^*$  individually, one process parameter is set as a constant value while the other changes. As shown in Figure 4.14, to investigate the effect of  $v^*$ individually,  $H^*$  is set as 1.5 while  $v^*$  changes from 0 to 1.2. As shown in Figure 4.15, to investigate the effect of  $H^*$  individually,  $v^*$  is set as 1.2 while  $H^*$  changes from 0 to 1.5. The deposition status starts from over-deposition to pressed-deposition and finally to freeformdeposition when  $v^*$  and  $H^*$  increase as shown in Figure 4.14 and Figure 4.15. The effect of  $v^*$  on width and height is influenced by its deposition status and is summarized as: width decreases with  $v^*$  in pressed-deposition and freeform-deposition; height remains the same with  $v^*$  in pressed-deposition while decreases with  $v^*$  in freeform-deposition. The effect of  $H^*$  on width and height is influenced by its deposition status and is summarized as: width decreases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition.



Figure 4.14 Effect of  $v^*$  on width and height when  $H^*$  is set as a constant value ( $H^*$  is set as 1.5 in the two charts): (a) width; (b) height



Figure 4.15 Effect of  $H^*$  on width and height when  $v^*$  is set as a constant value ( $v^*$  is set as 1.2 in the two charts): (a) width; (b) height

# 4.5 Numerical simulation of deposited corners

# 4.5.1 Numerical Modeling

The OpenFOAM v1912 is used to realize the numerical simulation of the 3D profile of deposited corners as plotted in Figure 4.16. In the numerical simulation, OpenFOAM v1912 is used to build geometrical model, generate meshes, determine boundary conditions and solve

governing equations. After numerical simulation in OpenFOAM v1912, ParaView is used to build visualizations and analyze simulation data.



Figure 4.16 Numerical modeling of 3D profile of deposited corners: (a) 3D geometrical model; (b) generated meshes; (c) velocity condition in substrates; (d) initial condition of phase fraction

#### (1) Geometrical model

The route of modeling of deposited corners of any angle in the proposed numerical simulation is to construct two computing areas, and simulate the corner of any angle by applying velocities of the same magnitude and different directions with the corner angle as the velocity direction angle to the substrates of the two computing areas. As shown in Figure 4.16 (a), the geometrical model consists of two areas named as area 1 and area 2 where joint surface 1 in area 1 (Figure 4.17 (a)) and joint surface 2 in area 2 (Figure 4.18 (a)) are merged to combine area 1 and area 2 into a complete model. As shown in Figure 4.17 (a), in area 1, the boundary

surfaces include inlet, nozzle inner wall, nozzle outer wall, nozzle bottom wall, air, joint surface 1 and substrate 1. As illustrated in Figure 4.17 (b), the critical parameters of area 1 include the inner diameter of nozzle  $d_n$ , the outer diameter of nozzle  $D_n$ , the average velocity of ink in nozzle  $v_e$ , the nozzle length  $L_n$ , and the distance between nozzle bottom and substrate  $h \cdot v_e$  is calculated using Eq. (4.11) based on the conservation of mass.



Figure 4.17 Illustration of 3D geometrical model of area 1 in model of DF: (a) boundary surfaces; (b) critical parameters



Figure 4.18 Illustration of 3D geometrical model of area 2 in model of DF: (a) boundary surfaces; (b) critical parameters

As shown in Figure 4.18 (a), in area 2, the boundary surfaces include air, joint surface 2 and substrate 2. As illustrated in Figure 4.18 (b), the critical parameters of area 2 include the *h* and the  $L_n$ . Area 2 is divided into area 201 and area 202 according to the values of  $L_n$  and *h* along the height direction as shown in Figure 4.18 (b), where the area with the height of *h* from substrate 2 is area 202 and the rest is area 201.

#### (2) Generated meshes

As shown in Figure 4.16 (b), meshes are generated as cuboid grids with arc edges in the areas related to circular nozzle and as cuboid grids with all straight edges in the areas outside

the circular nozzle to realize a smooth and precise interface simulation between ink and air. As illustrated in Figure 4.19, to improve calculation efficiency and accuracy, meshes are refined in the region of deposited filaments including inner nozzle and area between nozzle bottom and substrate in area 1 (Figure 4.19 (a)) and area 201 in area 2 (Figure 4.19 (b)).



Figure 4.19 Illustration of generated meshes in: (a) area 1; (b) area 2

#### (3) Boundary conditions

Velocity boundary conditions include the average velocity of ink in nozzle  $v_e$  on inlet, the nozzle velocity  $\mathbf{v}_{n1}$  on substrate 1 and the nozzle velocity  $\mathbf{v}_{n2}$  on substrate 2. As illustrated in Figure 4.16 (c), to avoid the model becoming a complex dynamic-mesh model which needs a large amount of computational time, the position of nozzle is fixed in the model while the substrate 1 is applied with a velocity  $\mathbf{v}_{n1}$  and the substrate 2 is applied with a velocity  $\mathbf{v}_{n2}$  in the boundary setting respectively as the movements of the nozzle and substrates are relative to each other. The values of  $\mathbf{v}_{n1}$  and  $\mathbf{v}_{n2}$  are same. The angle of  $\mathbf{v}_{n1}$  and  $\mathbf{v}_{n2}$  models the angle of deposited corners with the value of  $\theta$ . The boundary conditions for the numerical simulation is summarized as in Table 4.9.

Name and physical meaning	Туре	Setting
Inlet	Inlet	Velocity is set as $v_e$
Nozzle inner wall; nozzle outer wall; nozzle bottom wall	No-slip boundary	No-slip
Air	InletOutlet boundary	Depended on dynamic calculation
Substrate 1	No-slip boundary	Velocity is set as $v_{n1}$
Substrate 2	No-slip boundary	Velocity is set as $v_{n2}$

Table 4.9 Boundary conditions for the numerical simulation of deposited corners

Figure 4.16 (d) presents the condition of phase fraction at the initial time which means the nozzle is filled with ink at the initial time, where red regime represents the ink and blue regime represents the air.

#### 4.5.2 Experimental verification

#### (1) Experimental setup

In order to validate the proposed numerical simulation of deposited corners, the selected ink Nivea Cr are is used in corner deposition experiments. The corner deposition experiments are setup same as Figure 4.9 using the piston driven DIW 3D printer TM-081 (Tobeca Company, France). To fully show the proposed simulation of deposited corners has the ability to simulate corners of any angle, the value of  $\theta$  is set from 30 ° to 150 ° with the interval of 15 °. Before printing, the substrate is leveled using the method proposed in [189] to reduce the influence of substrate levelness on printed filaments and corners. After printing, a ruler is put aside the deposited corner, and a camera Logitech 720p (Logitech, Swiss) which is installed on the printer is used to take photos of deposited corners with the ruler. The camera is calibrated using asymmetric circular grid pattern [110] to reduce the influence of lens distortion on measurements.

The photos are processed using the software Matlab to obtain the outline of deposited corners in real dimensions. In the image processing of experimental photos, the photo is transferred to grayscale and outline of deposited corner is obtained based on the use of canny edge detection; then outline in pixel coordinate is transferred into outline in real world coordinate by comparing the dimension of a pixel and the real dimension shown in ruler. Finally, the simulated and experimental outlines in real world coordinate are compared and the maximum distance deviation between simulated and experimental outlines (MDDSEO) of deposited corners is obtained in the software Matlab. The MDDSEO is used as the quantitative indicator to analyze the effectiveness of the simulation. All corner deposition experiments are repeated three times to reduce experimental random error. The MDDSEO of each corner angle is presented as the mean  $\pm$  standard deviation. Statistical analysis is performed using one-way analysis of variance (ANOVA) where statistical significance is defined as p\* <0.05.

#### (2) Parameters setting

Parameters in numerical simulations of deposited corners include parameters of material properties, critical parameters of geometrical model and process parameters. Parameters of material properties of the selected ink are obtained experimentally in Section 3.2.3 and are

listed in Table 3.1. For critical parameters of geometrical model, the values of  $d_n$ ,  $D_n$  and  $D_p$  are set as 0.84 mm, 1.22 mm, and 21.6 mm, which match the actual dimensions of the used DIW 3D printer in the experimental verification, respectively. As the nozzle length has no effect on  $v_e$  and the final deposited filaments and corners, the value of  $L_n$  is set as 2.44 mm which is smaller than practice nozzle length (18 mm) to reduce computational time.

Deposition status and the profile dimension of the deposited filaments are influenced by process parameters including  $v_e$ , h and the value of  $\mathbf{v}_{n1}$  and  $\mathbf{v}_{n2}$  [125, 188]. Based on the results of Section 3.3, process parameters are selected as:  $v_e = 6$  mm/s; h = 0.75 mm; the value of  $\mathbf{v}_{n1}$  and  $\mathbf{v}_{n2}$  is 4.8 mm/s. As shown in Figure 4.20, DF under this process parameters combination has a stable and regular 3D shape and cross-sectional profile using the numerical simulation of DF proposed in Section 4.4. Finally, to model deposited corners of any angle, the value of  $\theta$  is set from 30° to 150° with the interval of 15° in numerical simulations and experiments to validate the numerical simulation of deposited corners of any angle.



Figure 4.20 Simulated DF under the selected process parameters combination: (a) 3D profile; (b) cross-sectional profile

### (3) Results

The simulation calculation times of corner when the value of  $\theta$  is set from 30° to 150° are listed in .

	20.9	<u>(0</u> °	000	1200	1509	
Corner angle	30°	60°	90°	120*	150*	
Simulation time/mins	116	172	145	100	65	

Table 4.10 Simulation calculation time of corner under different corner angles

The 3D profile and top view of simulated deposited corners and top view of three-times experimental results for deposited corners where the value of  $\theta$  is set from 30° to 150° with

the interval of 15 ° are represented in Figure 4.21. Comparison of simulation and experimental results is conducted in the software Matlab using image processing and plotted in Figure 4.22. In Figure 4.22, the green area represents the simulation result of deposited filaments and corners; the grey area represents the substrate; the red, yellow and purple dashed lines represent experimental outlines of deposited corners in the first, second and third test, respectively; the blue solid line represents the MDDSEO of deposited corners.



Figure 4.21 Simulation and experimental results of deposited corners where the value of corner angle is set from 30 °to 150 °with the interval of 15 °



Figure 4.22 Comparison of simulation and experimental results of deposited corners when is set as: (a) 30 °; (b) 45 °; (c) 60 °; (d) 75 °; (e) 90 °; (f) 105 °; (g) 120 °; (h) 135 °; (i) 150 °

As shown in Figure 4.22, the simulation results of deposited straight filaments and the corner angles formed by two straight filaments fit experimental results well. For outlines of the deposited corners, the MDDSEO is used as indicator to illustrate the comparison between simulation and experimental results quantitatively. Based on the marked MDDSEO in Figure 4.22, MDDSEO of deposited corners under different corner angles are summarized in Table 4.11 and Figure 4.23. As shown in Table 4.11 and Figure 4.23, the maximum value and minimum value of MDDSEO is 1.06  $\pm$ 0.06 mm and 0.09  $\pm$ 0.01 mm when  $\theta$  is set as 30 ° and 150 °, respectively; and the MDDSEO decreases as  $\theta$  increases. Thus, the proposed numerical simulation is validated as an effective method to model deposited corners of any angle as the simulated corner angles fit experimental angles well and the maximum value of MDDSEO is 1.06  $\pm$ 0.06 mm.

Corner angle ( )	30	45	60	75	90	105	120	135	150
MDDSEO (mm)	$\begin{array}{c} 1.06 \ \pm \\ 0.06 \end{array}$	$\begin{array}{c} 0.84 \ \pm \\ 0.04 \end{array}$	$0.45 \pm 0.02$	$0.41 \pm 0.02$	${0.33 \ \pm \\ 0.05}$	0.16 ± 0.01	$0.14 \pm 0.01$	$0.13 \pm 0.01$	$\begin{array}{c} 0.09 \ \pm \\ 0.01 \end{array}$

Table 4.11 Maximum distance deviation between simulated and experimental outlines(MDDSEO) of deposited corners



Figure 4.23 Maximum distance deviation between simulated and experimental outlines (MDDSEO) of deposited corners under different corner angles

However, the MDDSEO of corners is larger than MDDSEO of straight filaments where the maximum value of MDDSEO is 1.06 ±0.06 mm for corners while the maximum value of MDDSEO is less than 0.20 mm for straight filaments, which means prediction accuracy of corners is inferior than that of straight filaments in the simulation. The reason for this phenomenon is due to the difference between the nozzle velocity applied on substrate in numerical simulation and real nozzle velocity in experiments only for the corner region. As shown in Figure 4.24 (a), the trajectory of nozzle velocity applied on substrate is from point A to point B and then from point B to point C. As illustrated in Figure 4.24 (b) and Figure 4.24 (c), in numerical simulation, the value of velocity on substrate along x axis is a constant  $v_{nx}$ along the trajectory, and the value of velocity on substrate along y axis can change from  $v_{ny}$  to  $-v_{ny}$  at point B immediately. In practice experiments, the nozzle cannot change velocity immediately and need a uniform deceleration and uniform acceleration process to change nozzle velocity direction [190] and the acceleration depends on the firmware of the DIW 3D printer [152]. As shown in Figure 4.25 (a), the trajectory of nozzle velocity applied on substrate is divided into 4 stages as follows where detail velocity profile along x axis and y axis is plotted in Figure 4.25 (b) and Figure 4.25 (c), respectively:

- Point A to point B<sub>1</sub>: uniform velocity process;
- Point B<sub>1</sub> to point B<sub>2</sub>: uniform deceleration process;
- Point B<sub>2</sub> to point B<sub>3</sub>: uniform deceleration process;
- Point B<sub>3</sub> to point C: uniform velocity process.

Comparing Figure 4.24 and Figure 4.25, the difference of nozzle velocity between numerical simulation and real experiment leads to the simulation prediction error in corner regions. As shown in Figure 4.23, the MDDSEO of corners decreases as the corner angle increases which means that the effect of difference of nozzle velocity between numerical simulation and real experiment on deposited corners decreases as the corner angle increases.



Figure 4.24 Velocity profile on substrate in numerical simulation and design of G-code: (a) trajectory; (b) value of velocity on substrate along x axis; (c) value of velocity on substrate along y axis



Figure 4.25 Velocity profile on substrate in actual corner deposition experiments: (a) trajectory; (b) value of velocity on substrate along x axis; (c) value of velocity on substrate along y axis

# 4.6 Conclusion

In this chapter, numerical simulations of the most basic elements in DIW including FEF, DF and deposited corner are proposed and experimental verifications are conducted to verify the proposed numerical simulations. Based on the proposed numerical simulations, process analyses of DIW are conducted.

For numerical simulation of FEF, a numerical model of FEF is established with numerical simulation method and then the FEF is evaluated based on this model. Two evaluation indicators, mean diameter and stability, are proposed to evaluate the FEF. The selected ink Nivea Cr ème is used to verify the method. The established numerical model of FEF is verified as the shape in simulation is in accordance with experimental results and the diameter prediction accuracy is better than 0.08 mm. After experimental verification, the model and evaluation indicators are used to deal with the two questions in process analysis for FEF in DIW as follows:

(1) Analyze effect of the piston velocity on FEF: there is a minimum piston velocity, 2 mm/s for Nivea Cr are for setting of  $v_e$ , to produce continuous and stable FEF; mean diameters of FEF decrease with increasing piston velocity. Stability decreases firstly and then increases as piston velocity increases;

(2) Find suitable printable windows for process parameters: printable window of setting of  $v_e$  is 5 mm/s-15 mm/s for Nivea Cr ème.

For numerical simulation of DF, the detailed influence of process parameters on the deposition status and profile dimension has not been fully quantitatively characterized in the previous numerical prediction works for the DF of direct ink writing. In this chapter, the effect of process parameters on the deposition status and profile dimension has been quantified based on numerical prediction. An improved 3D numerical model is established by using VOF method and by considering the overall ink material properties. The improved 3D numerical model overcomes the problem of previous simplified 2D models in predicting cross-section and the shortcoming of previous 3D numerical models in ignoring important material properties such as surface tension coefficient and static contact angle which limit the prediction accuracy. Critical process parameters are identified as the dimensionless nozzle velocity and the dimensionless height.

Based on the numerical prediction, the deposition status is characterized into three types named over-deposition, pressed-deposition and freeform-deposition and the profile dimension under each deposition status is predicted. The effectiveness of the numerical prediction for the deposited filaments is validated as the simulated deposited statues dividing results are consistent with the experimental results and are also consistent with the idealized results. The prediction accuracy of the numerical prediction for the profile dimension is verified as the maximum relative errors of width and height between experimental and simulated results are 10.13% and 7.37% respectively which are significantly improved as compared with the reported values of 20% and 28% in the literature. The maximum relative error of the numerical prediction appears at the edge of the printable window.

Based on the numerical prediction, the effects of the process parameters on DF are also investigated. The deposition status starts from over-deposition to pressed-deposition and finally to freeform-deposition when  $V^*$  and  $H^*$  increase while average the velocity of ink in nozzle has no significant effect on the deposition status and profile dimension. The deposition status should be taken into consideration for the effect of process parameters on the profile dimension: the width decreases with  $V^*$  in pressed-deposition and freeform-deposition; the height remains the same with  $V^*$  in pressed-deposition while decreases with  $V^*$  in freeformdeposition; the width decreases with  $H^*$  in pressed-deposition while remains the same with  $H^*$ in freeform-deposition; the height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$ in freeform-deposition. The proposed numerical simulation and process analysis for DF characterize the deposition status and study the profile dimension in each deposition status based on the use of numerical prediction. The numerical simulation of DF suggests a material-saving and effective numerical prediction for the deposition status and profile dimension of the DF and the investigation of the effects of process parameters in DIW. It also provides a viable basis for the future work on the elaboration of numerical modeling of the overall DIW 3D printing process.

For numerical simulation of deposited corners, the previous research works for numerical simulation of deposited corners could only achieve the corner simulation under the condition of small angle and failed to realize corner simulation of any angle. In this chapter, an improved 3D numerical simulation of deposited corners is established by using VOF method and by considering the overall ink material properties. The improved 3D numerical simulation overcomes the limitation of the previous work and realizes deposited corner modeling of any angle by constructing two calculation areas where two nozzle velocities with the corner angle are applied on the substrates of two calculation areas. The effectiveness of the proposed numerical model is validated through corners deposition experiments using the selected ink in a DIW 3D printer as the simulated corner angles fit experimental angles well and the maximum value of MDDSEO is  $1.06 \pm 0.06$  mm. It is observed that the simulation accuracy in corners is inferior than that in filaments. The reason for this phenomenon is due to the difference between the nozzle velocity applied on substrate in numerical simulation and real nozzle velocity in experiments only for the corner region as the nozzle needs a uniform deceleration and uniform acceleration process to change nozzle velocity direction in practice printing. The MDDSEO of deposited corners decreases as the corner angle increases.

The numerical simulations of FEF, DF and deposited corners provides an effective numerical simulation for the modeling outputs in DIW.It could be used in DIW process analyses work including the printability evaluation of new prepared inks, the process parameters optimization and the establishment of digital twin. They also provide a viable basis for the future work on the elaboration of numerical modeling of the overall DIW 3D printing process.
### **Chapter 5: Conclusion and perspectives**

### 5.1 Conclusion

The process understanding and analysis of DIW have not been fully studied, which limits the manufacturing accuracy and application promotion of this technique. To solve this problem, it is of critical to do research on process analysis for DIW to fully understand this process and improve the usability of DIW. Numerical simulation is one of the most powerful tools in process analysis in AM. Process analysis based on numerical simulations has advantages in saving material/trial time and easily capturing critical process parameters value which are difficult obtained by experimental measurements. The research on process modeling and analysis of DIW based on numerical simulations will provide important support for the development and guidance of DIW. However, there is currently few systematic work on process modeling and analysis based on numerical simulations for DIW. To bridge this gap, this thesis proposes a process modeling and analysis for DIW based on numerical simulations.

In chapter 2, a systematic literature review of DIW is conducted firstly to summarize features, development, challenges and solutions for challenges of DIW and an insufficiently solved problem - difficulty to quickly find suitable process parameters for the prepared ink - is determined as the research question of this thesis. To solve the research question, process modeling and analysis for DIW is selected as the solution. Afterwards, a literature review of process modeling and analysis for DIW is conducted. Inputs and outputs of process modeling are summarized and numerical process modeling methods are selected as the most suitable method for process modeling and analysis based on numerical simulations for DIW. Based on the review, the objective of this thesis is determined as: to propose a process modeling and analysis for DIW based on numerical simulations.

In chapter 3, the ink Nivea Cr ème and a piston-driven DIW 3D printer are chosen to verify the proposed numerical simulations. Before numerical simulation, ink material properties are characterized and optimal process parameters setting is selected to provide the basis for modeling inputs. For ink material properties characterization, density, surface tension, static contact angle and rheology properties are obtained for the used ink. For process parameters selection, the DIW process parameters are identified through process analyses and a two-step method is proposed to optimize DIW process parameters for dimensional accuracy and analyze the significance of each process parameter. Experimental verifications verify the proposed process parameters selection method and the method robustness on other shapes; parameter adaptability in 3D parts printing from printed layers' analyses for the proposed method and parameter adaptability in constructs fabricated as 100% infill or with porosities.

In chapter 4, numerical simulations of the most basic elements in DIW including FEF, DF and deposited corner are proposed and experimental verifications are conducted to verify the proposed numerical simulations. Based on the proposed numerical simulations, process analyses of DIW are conducted.

For numerical simulation of FEF, the established numerical model of FEF is verified as the shape in simulation is in accordance with experimental results and the diameter prediction accuracy is better than 0.08 mm. Process analysis based on the numerical simulation of FEF shows that: 1) there is a minimum piston velocity, 2 mm/s for Nivea Cr ane for setting of  $v_e$ , to produce continuous and stable FEF; 2) mean diameters of FEF decrease with increasing piston velocity and stability decreases firstly and then increases as piston velocity increases; 3) suitable printable windows for setting of  $v_e$  is 5 mm/s-15 mm/s for Nivea Cr ane.

For numerical simulation of DF, the effect of process parameters on the deposition status and profile dimension has been quantified based on numerical prediction of DF. An improved 3D numerical model is established by using VOF method and by considering the overall ink material properties. The improved 3D numerical model overcomes the problem of previous simplified 2D models in predicting cross-section and the shortcoming of previous 3D numerical models in ignoring important material properties such as surface tension coefficient and static contact angle which limit the prediction accuracy. Critical process parameters are identified as the dimensionless nozzle velocity and the dimensionless height. Based on the numerical prediction, the deposition status is characterized into three types named overdeposition, pressed-deposition and freeform-deposition and the profile dimension under each deposition status is predicted. The effectiveness of the numerical prediction for the DF is validated as the simulated deposited statues dividing results are consistent with the experimental results and are also consistent with the idealized results.

The prediction accuracy of the numerical prediction for the profile dimension is verified as the maximum relative errors of width and height between experimental and simulated results are 10.13% and 7.37% respectively which are significantly improved as compared with the reported values of 20% and 28% in the literature. The maximum relative error of the numerical prediction for the profile dimension appears at the edge of the printable window. Based on the numerical prediction, the effects of the process parameters on DF are also investigated. The deposition status starts from over-deposition to pressed-deposition and finally to freeform-deposition when  $V^*$  and  $H^*$  increase while average the velocity of ink in nozzle has no significant effect on the deposition status and profile dimension. The deposition status should be taken into consideration for the effect of process parameters on the profile dimension: the width decreases with  $V^*$  in pressed-deposition and freeform-deposition; the height remains the same with  $V^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; the width decreases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; the height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; the height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; the height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; the height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; the height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition; the height increases with  $H^*$  in freeform-deposition; the height increases with  $H^*$  in pressed-deposition while remains the same with  $H^*$  in freeform-deposition;

For numerical simulation of deposited corners, the previous research works for numerical simulation of deposited corners could only achieve the corner simulation under the condition of small angle and failed to realize corner simulation of any angle. An improved 3D numerical simulation of deposited corners is established by using VOF method and by considering the overall ink material properties. The improved 3D numerical simulation overcomes the limitation of the previous work and realizes deposited corner modeling of any angle by constructing two calculation areas where two nozzle velocities with the corner angle are applied on the substrates of two calculation areas. The effectiveness of the proposed numerical model is validated through corners deposition experiments using the selected ink in a DIW 3D printer as the simulated corner angles fit experimental angles well and the maximum value of MDDSEO is  $1.06 \pm 0.06$  mm. It is observed that the simulation accuracy in corners is inferior than that in filaments and the MDDSEO of deposited corners decreases as the corner angle increases.

In conclusion, this thesis determines the research objective through systematic literature reviews and realize the objective by ink material property characterization, process parameters selection, numerical simulations, experimental verification and process analysis. This thesis suggests an effective numerical simulation for the modeling outputs in DIW which could be used in DIW process analyses work including the printability evaluation of new prepared inks, the process parameters optimization and the establishment of digital twin, which is helpful for the process understanding and analysis of DIW.

### **5.2 Perspectives**

Following the works presented in Chapter 1-4, many other perspectives can be envisaged. Among those I hope to follow are:

For process parameters selection, there is a limitation in quantitative analysis of printed objects (parts) and the thesis does not obtain a quantitative relationship between input and output based on experimental method. Future work will conduct a quantitative evaluation for printed objects using computer vision method and a quantitative relationship between input and output will be proposed based on the quantitative data using response surface methodology.

For numerical simulations of DIW, the thesis does not establish numerical simulations of printed layers and 3D parts. Future work will establish numerical simulations of printed layers and 3D parts to realize modeling of all outputs for DIW including FEF, DF, deposited corners, printed layers and 3D parts.

For process analysis of DIW, the thesis does not fully analyze the process in the printability evaluation of new prepared inks, the process parameters optimization and the establishment of digital twin. Future work will conduct a complete process analyses work including the printability evaluation of new prepared inks, the process parameters optimization and the establishment of digital twin, which is helpful for the process understanding and analysis of DIW.

Non-planar substrates and the use of multi-axis robots are important direction for DIW owing to their ability to build more complex geometries. Future work will study the non-planar substrates and the use of multi-axis robots.

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# Appendices

#### Appendix A Derivation for the relationship between $R_w$ and W

As illustrated in Figure A1, the gravity of printed layer could be calculated as:

$$W = A_f \cdot \frac{Lx}{d_l} \cdot Lx \cdot Ly \cdot \rho \cdot g \tag{A. A1}$$

Where *w* is the weight of printed layer;  $A_f$  is the cross section area of filament on the substrate; Lx and Ly are designed dimension in x and y direction respectively;  $d_i$  is distance between lines;  $\rho$  is the material density; *g* is the gravity accelerate.



Figure A 1. Illustration of the relationship between  $R_{W}$  and W

Meanwhile,

$$\frac{1}{4}\pi D_p^2 \cdot v_p = A_f \cdot v_e \tag{A. A2}$$

$$v_p = \frac{1}{V^*} \cdot \frac{D_p^2}{d_s^2} \cdot v_n$$
 (A. A3)

$$d_l = R_W \cdot \overline{w}_O \tag{A. A4}$$

Where all variables in Eq. (A. A2) -(A. A4) have been defined in Section 3.3.2.

Combining Eq. (A. A1) -( A. A4), the relationship between  $R_w$  and w is obtained as follows:

$$W = \frac{1}{4}\pi \frac{D_p^4}{d_s^2} \cdot \left(Lx\right)^2 \cdot Ly \cdot \rho \cdot g \cdot \frac{1}{\overline{w}_o \cdot R_w}$$
(A. A5)

#### Appendix B Detailed information for interaction effect tests

Two-factor interaction effects are considered. In interaction effect tests, one factor of  $v_n$ ,  $v^*$  and  $H^*$  is fixed and the remaining two factor are changed to print lines. As listed in Table A 1, in interaction effect test for  $v_n \times V^*$ ,  $H^*$  is fixed in 0.9;  $v^*$  is changed as 1, 0.8 and 0.6 for 5 mm/s and 11 mm/s of  $v_n$ . As listed in Table A 2, in interaction effect test for  $v_n \times H^*$ ,  $v^*$  is fixed in 0.8;  $H^*$  is changed as 0.6, 0.9 and 1.2 for 5 mm/s and 11 mm/s of  $v_n$ . As listed in Table A 3, in interaction effect test for  $v^* \times H^*$ ,  $v_n$  is fixed in 8 mm/s;  $H^*$  is changed as 0.6, 0.9 and 1.2 for 1 and 0.6 of  $v^*$ .

Process parameters setting		
$v_n/(\text{mm/s})$	$V^{*}$	$H^{*}$
5	1	0.9
5	0.8	0.9
5	0.6	0.9
11	1	0.9
11	0.8	0.9
11	0.6	0.9
	$v_n / (mm/s)$ 5         5         5         11         11         11         11	$v_n$ /(mm/s) $V^*$ 5       1         5       0.8         5       0.6         11       1         11       0.8         11       0.6

Table A 1 Process parameters setting of interaction effect test for  $v_n \times V^*$ 

Experiment number	Process parameters setting			
	$v_n/(\text{mm/s})$	$V^*$	$H^{*}$	
S3-1	5	0.8	0.6	
\$3-2	5	0.8	0.9	
\$3-3	5	0.8	1.2	
S4-1	11	0.8	0.6	
\$4-2	11	0.8	0.9	
S4-3	11	0.8	1.2	

*Table A 2 Process parameters setting of interaction effect test for*  $v_n \times H^*$ 

Experiment number	Process parameters setting			
	$v_n/(\text{mm/s})$	$V^*$	$H^{*}$	
85-1	8	1	0.6	
\$5-2	8	1	0.9	
\$5-3	8	1	1.2	
S6-1	8	0.6	0.6	
S6-2	8	0.6	0.9	
86-3	8	0.6	1.2	

#### **Appendix C List of publications**

### **Journal articles:**

- [1] Yongqiang Tu, Javier A. Arrieta-Escobar, Alaa Hassan, et al. Optimizing Process Parameters of Direct Ink Writing for Dimensional Accuracy of Printed Layers [J]. 3D Printing and Additive Manufacturing, 2021, published online. DOI: 10.1089/3dp.2021.0208
- [2] Yongqiang Tu, Alaa Hassan, Javier A. Arrieta-Escobar, et al. Modeling and evaluation of freeform extruded filament based on numerical simulation method for direct ink writing
   [J]. The International Journal of Advanced Manufacturing Technology, 2022, 120: 3821-3829. DOI: 10.1007/s00170-022-08999-3
- [3] Yongqiang Tu, Alaa Hassan, Ali Siadat, et al. Numerical simulation and experimental validation of deposited corners of any angle in direct ink writing [J]. The International Journal of Advanced Manufacturing Technology, 2022, 123: 559-570. DOI: 10.1007/s00170-022-10195-2
- [4] Yongqiang Tu, Alaa Hassan, Ali Siadat, et al. Analytical modeling of deposited filaments for high viscosity material-based piston-driven direct ink writing [J]. The International Journal of Advanced Manufacturing Technology, 2022, 123: 3387-3398. DOI: 10.1007/s00170-022-10511-w

### **Conference articles:**

- [1] Yongqiang Tu, Javier A. Arrieta-Escobar, Alaa Hassan, et al. Predictive modeling of extruded filament in the air for bioink in direct ink writing using numerical simulation [C]. Procedia CIRP, 2022, 112(4): 394-399. DOI: 10.1016/j.procir.2022.09.026
- [2] Yongqiang Tu, Alaa Hassan, Ali Siadat, et al. Multi-objective optimization based viscosity prediction for inks in direct ink writing numerical simulations [C]. Intelligent Networked Things, CINT 2022, Communications in Computer and Information Science, 2022, 1714: 147-157. DOI: 10.1007/978-981-19-8915-5\_13
- [3] Yongqiang Tu, Huiyun Gong, Alaa Hassan, et al. Computer vision-based evaluation of dimensional accuracy for MEAM in new product development [C]. Accepted. // The CIRP Design conference, 2023, Sydeny, NSW, Australia.

# Yongqiang TU Process modeling and analysis for direct ink writing based on numerical simulations

# R ésum é

L'ériture directe àl'encre (DIW) est l'une des techniques de fabrication additive (FA) les plus populaires ces derni àres ann és. DIW appartient à la FA à extrusion de mat ériaux (MEAM) et elle pr ésente des avantages exceptionnels en termes de compatibilit é des mat ériaux et de flexibilit é de l'équipement par rapport aux autres techniques FA. Cependant, la compr énension et l'analyse du processus de DIW n'ont pas é é enti àrement étudi és, ce qui limite la pr écision de fabrication et la promotion de l'application de cette technique. La simulation num érique est l'une des outils les plus puissants d'analyse de processus en FA. La recherche sur la mod élisation des processus et l'analyse de DIW bas é sur des simulations num ériques fournira un soutien important pour le d éveloppement et l'orientation de DIW. Cependant, il existe actuellement peu de travaux syst ématiques sur la mod élisation et l'analyse des processus bas és sur des simulations num ériques pour DIW. Pour combler cette lacune, l'objectif de cette th èse est de faire des recherches sur la mod élisation et l'analyse des processus pour DIW bas é sur des simulations num ériques. Cette th èse propose des simulations num ériques efficaces bas és sur la m éhode VOF (Volume OF Fluid) pour la mod élisation des sorties dans DIW et vérifie les simulations num ériques par v érification exp érimentale. L'analyse des processus est effectu é sur la base des simulations num ériques propos és, ce qui est utile pour la compr énension et l'analyse des processus de DIW.

**Mots cl és:** Ecriture directe à l'encre, Simulation num érique, Analyse de processus, Volume de fluide, Extrusion de mati ère

# R ésum é en anglais

Direct ink writing (DIW) is one of the most popular additive manufacturing (AM) techniques in recent years. DIW belongs to material extrusion AM (MEAM) and it has outstanding advantages in terms of material compatibility and equipment flexibility compared with other AM techniques. However, the process understanding and analysis of DIW have not been fully studied, which limits the manufacturing accuracy and application promotion of this technique. Numerical simulation is one of the most powerful tools in process analysis in AM. The research on process modeling and analysis of DIW based on numerical simulations will provide important support for the development and guidance of DIW. However, there is currently few systematic work on process modeling and analysis based on numerical simulations for DIW. To bridge this gap, the objective of this thesis is to do research on process modeling and analysis for DIW based on numerical simulations. This thesis suggests effective numerical simulations based on Volume Of Fluid (VOF) method for the modeling outputs in DIW and verifies the numerical simulations by experimental verification. Process analysis is conducted based on the proposed numerical simulations, which is helpful for the process understanding and analysis of DIW.

Keywords: Direct ink writing, Numerical simulation, Process analysis, Volume of fluid, Material extrusion