Practical Thermal Flow Analysis on Extrusion Molding Using 2.5D Finite Element Method

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HASL Co., Ltd, Japan

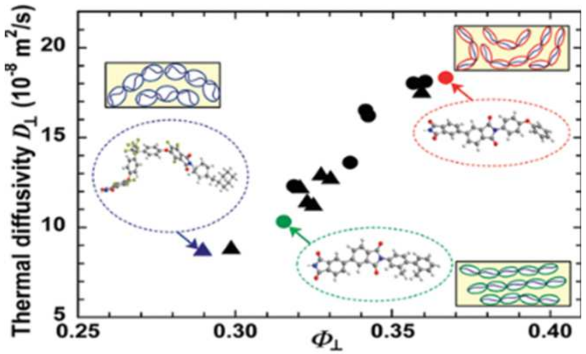
My Doctor Course Study (2007-2010)

Shinji Ando

Professor,
Tokyo Institute
of Technology

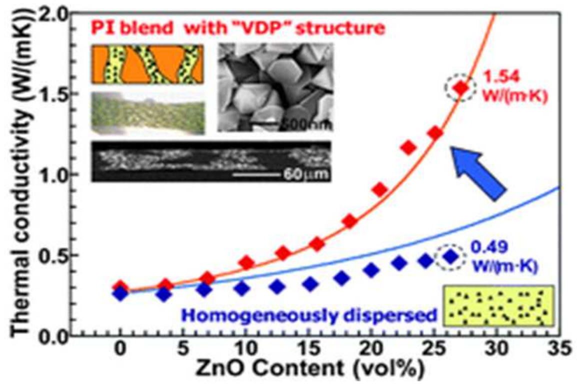
"Molecular Structure Dependence of Out-of-Plane Thermal Diffusivities in Polyimide Films",

D. Yorifuji; S. Ando, *Macromolecules,* 2010, *43*, 7583.



"Enhanced Thermal Conductivity over Percolation Threshold in Polyimide Blend Films Containing ZnO Nano-pyramidal Particles",

D. Yorifuji; S. Ando, *J. Mater. Chem.,* 2011, *21*, 4402.



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Shinichiro Tanifuji
Founder President,
2010 Aug. – 2024 Jan.
Advisor, 2024 Feb.-

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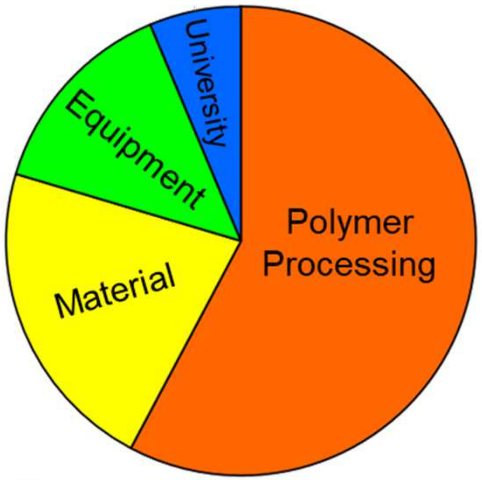
Executive Officer,
2019 Apr. – 2024 Jan.
President, 2024 Feb.-

Software Sales

Users



Our Developing Software

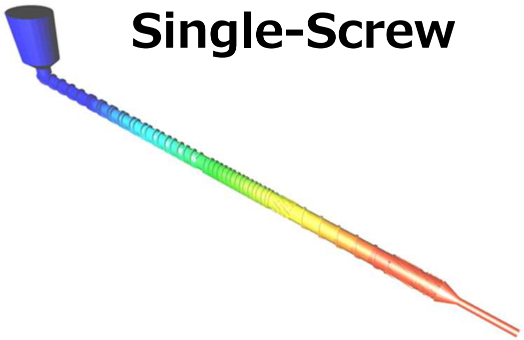
Thermal Flow Analysis on Extrusion Molding

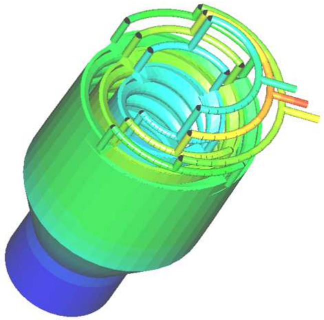
Upstream

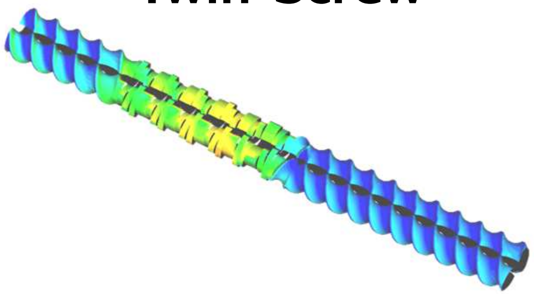
- Plasticize / Melt
- Knead / Mix

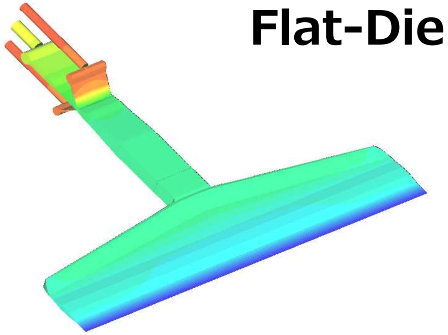
Downstream

- Shape
- Functionalize



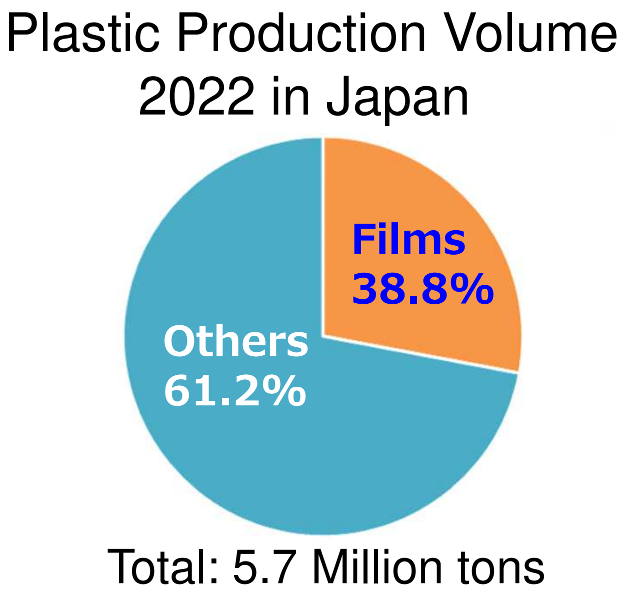


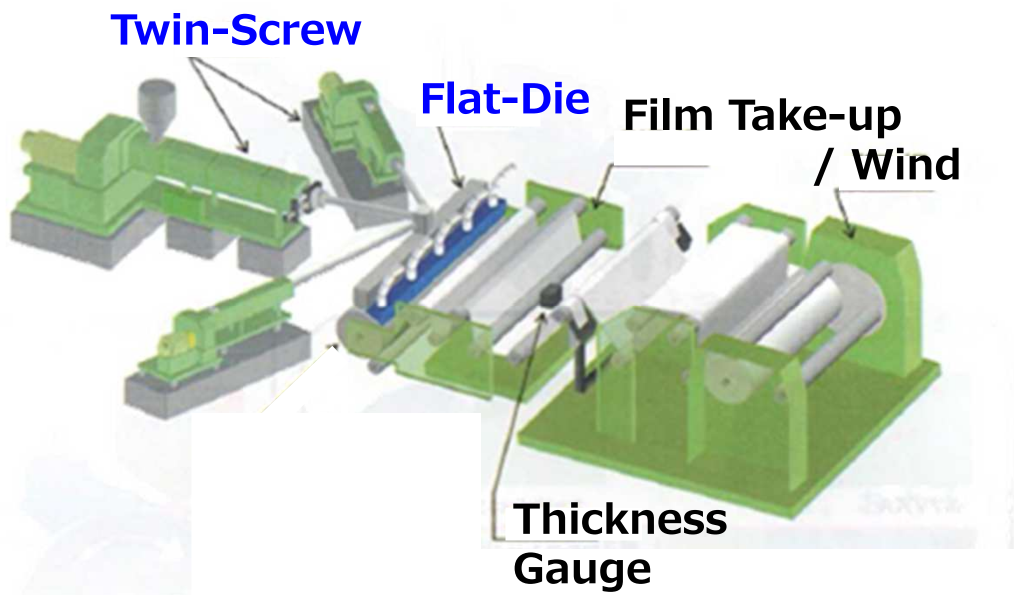


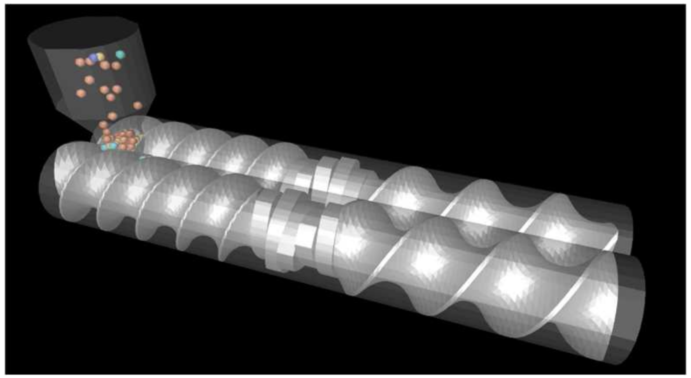


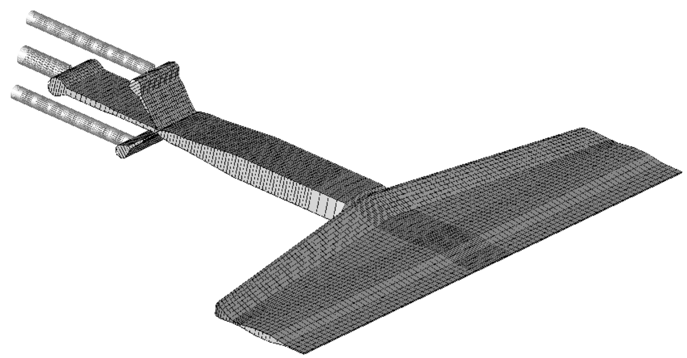
Today's Topic

Twin-Screw Extrusion / Multilayer Film Coextrusion



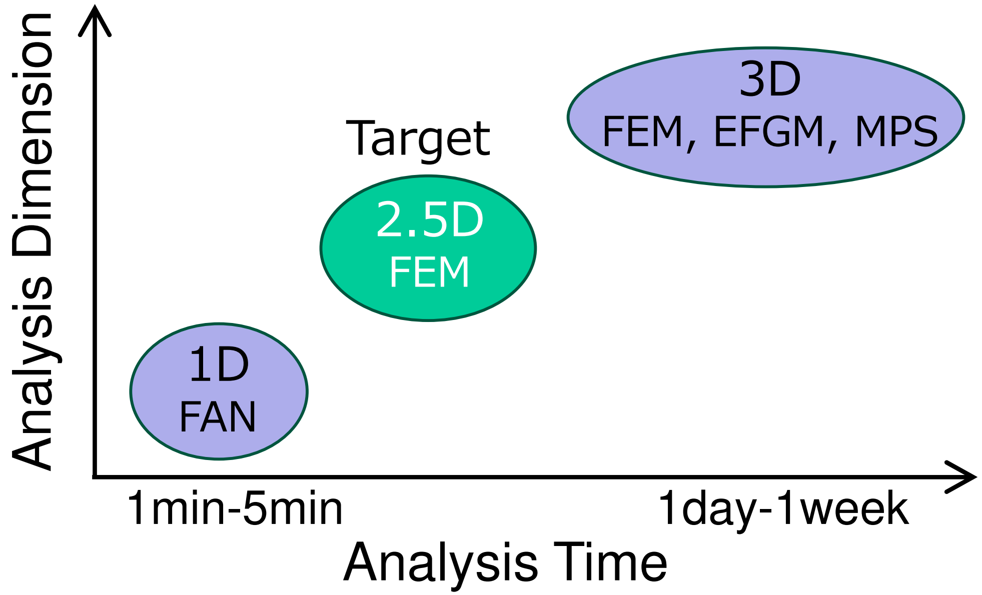




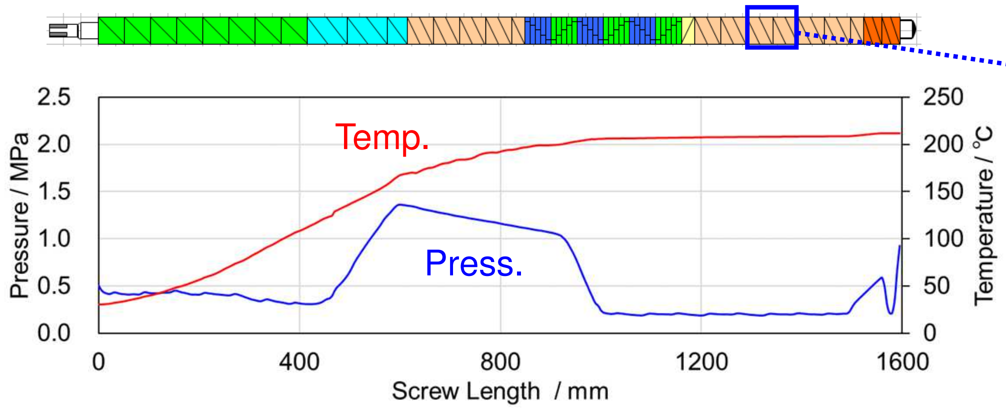


Agenda

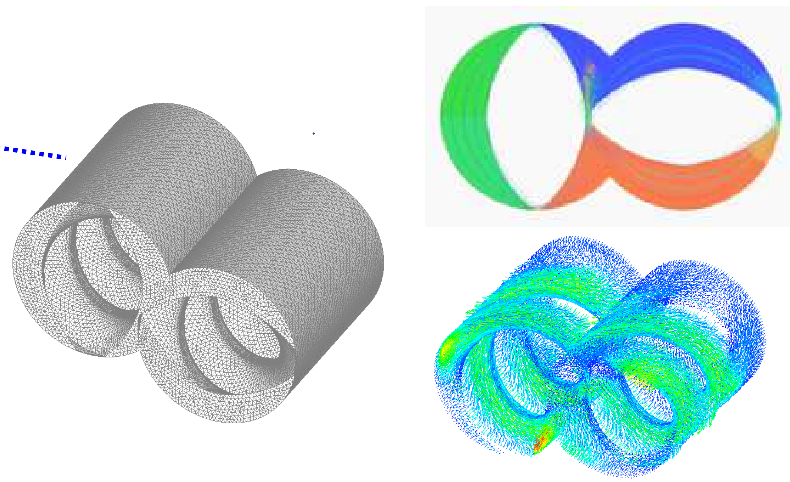
Development Target: 2.5D FEM



1D FAN (Flow Analysis Network)



3D FEM (Finite Element Method)

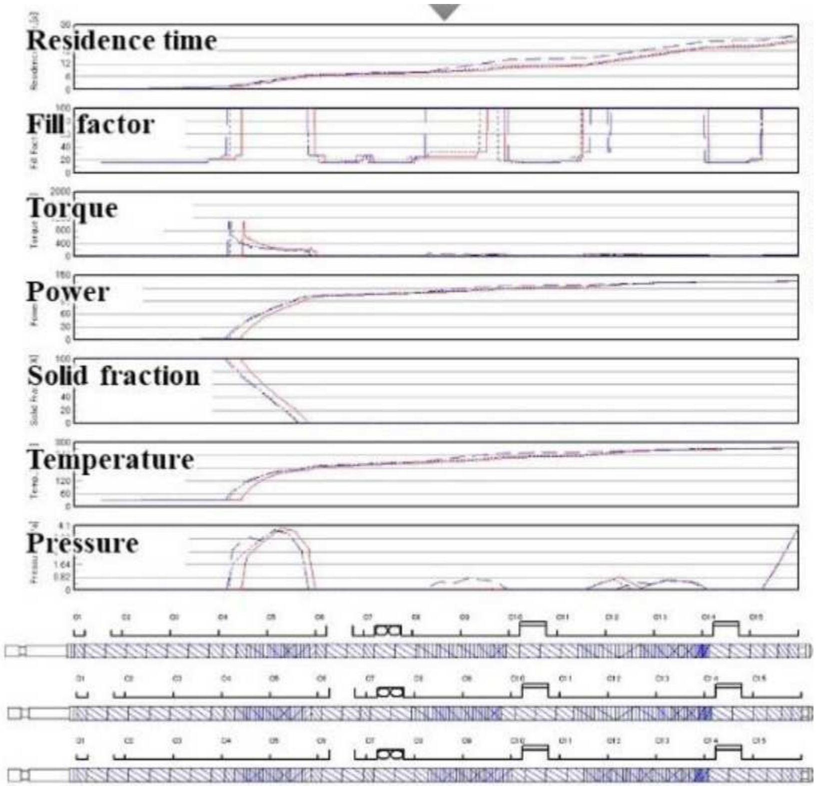


Reference of 1D and 3D Analysis

Annual Meeting of Japan Society of Polymer Processing, June 2024

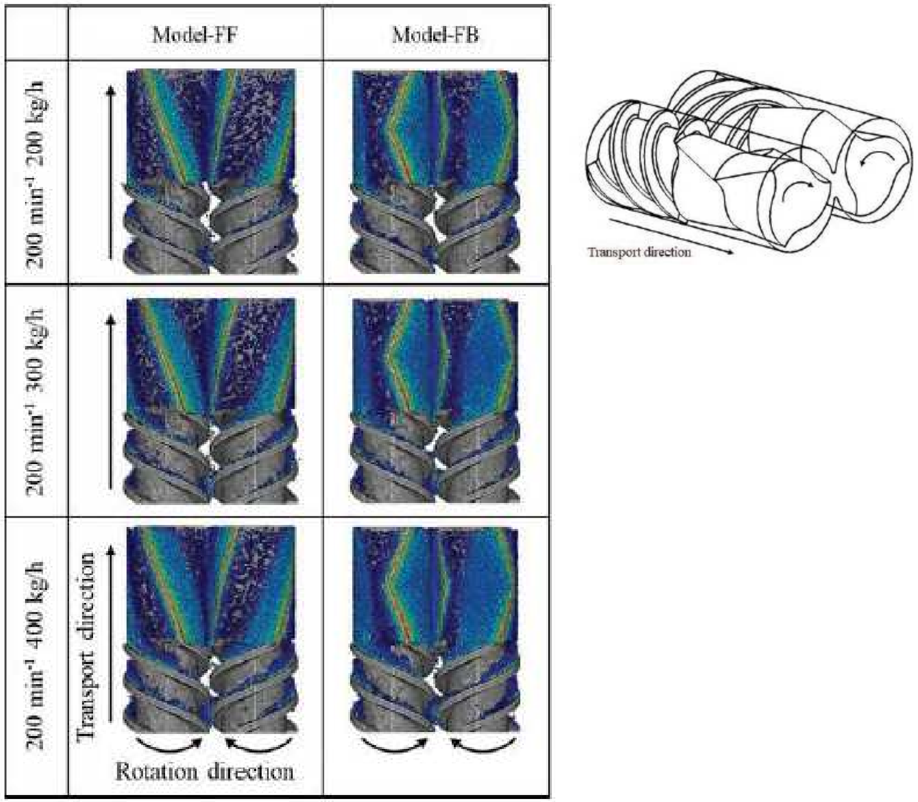
1D FAN

"Numerical Analysis of Resin Flow in the Twin Screw Extruder",
Y. Fukuzawa, I201 (2024)



3D EFGM

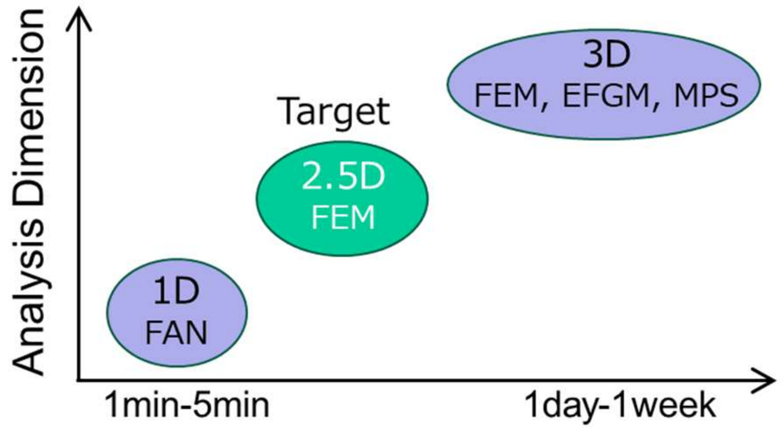
"Study on Melt Mixing of Polymeric materials in a Counter-Rotating Continuous Mixer Using Partially Filled Flow Simulation",
K. Sekiyama, et al., E206 (2024)



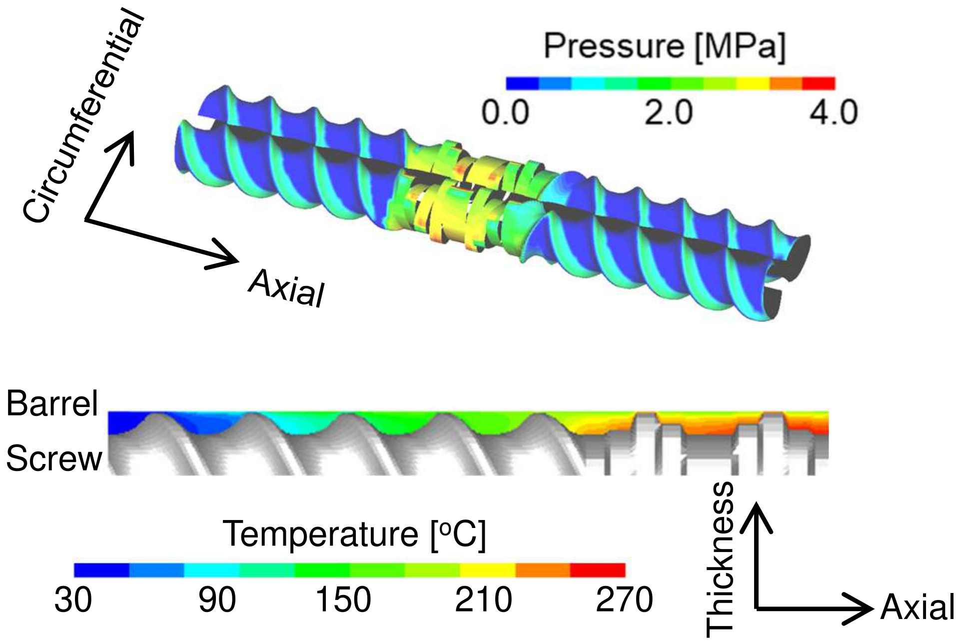
Key Technologies of 2.5D FEM for Practical Analysis

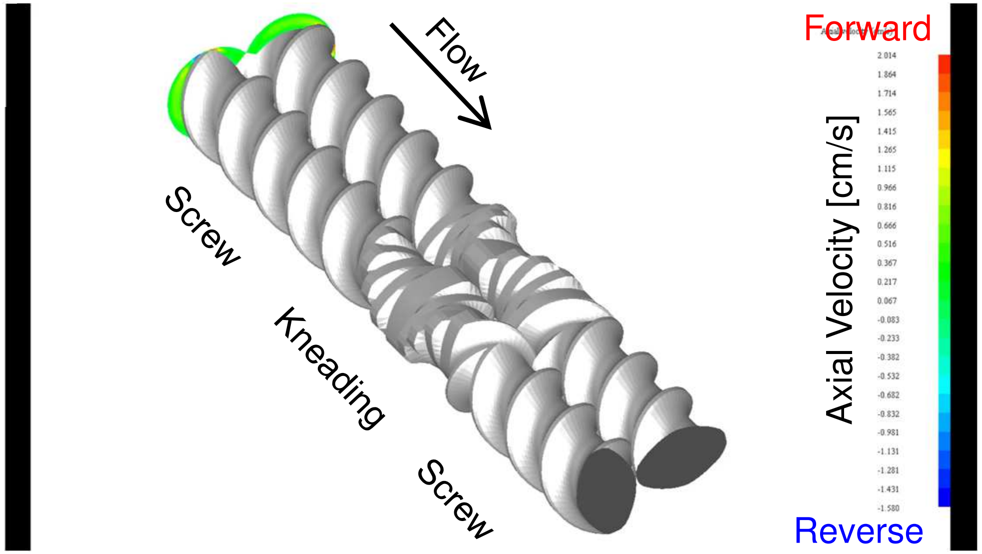
1. Modeling
   - No Need 3D CAD
   - User Friendly Input System

2. Analyzing
   - Overall Screw Length
   - Analysis Time: within One Hour



⇒ Visualization Results

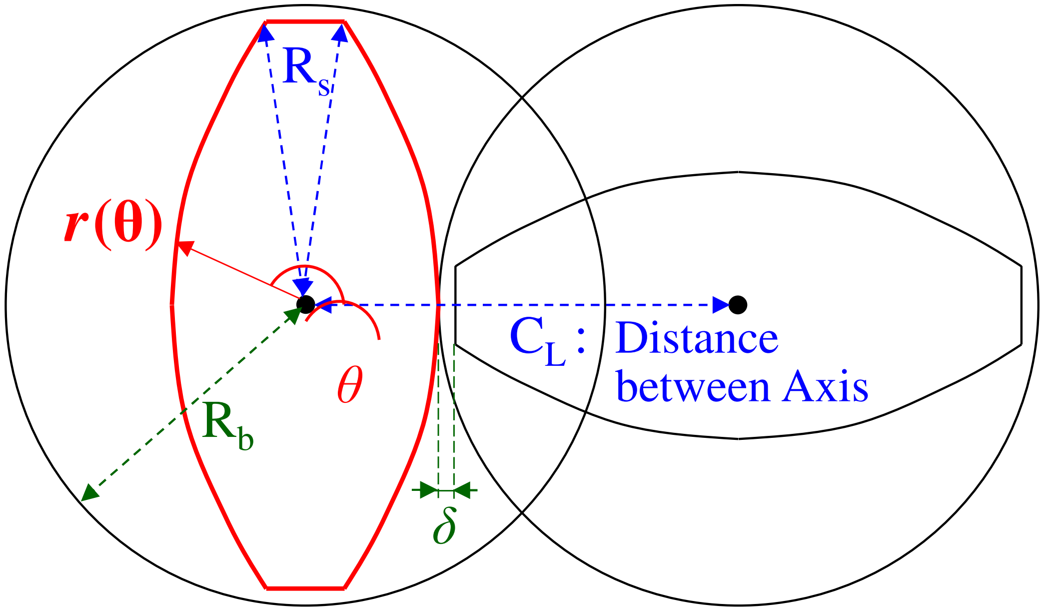


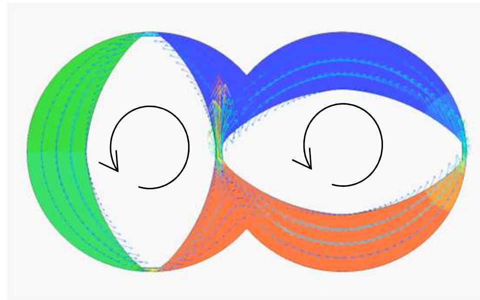


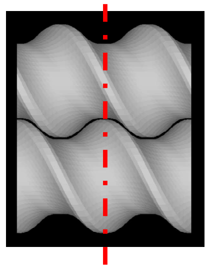
Key Technology 1: Modeling

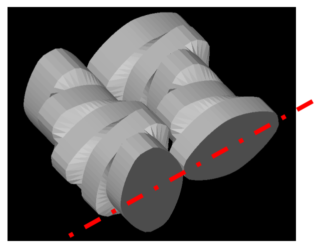
Cross Section of Fully Wiped Co-rotating Twin-Screw

$$r(\theta) = \sqrt{C_L^2 - R_s^2 \sin^2\theta} - R_s \cos\theta$$









Reference:
M. L. Booy, *Polym. Eng. Sci.*, **18**, 973 (1978).

Numerical Input of Model Information

GUI Form

Intermeshing Type

Intermeshing co-rotating

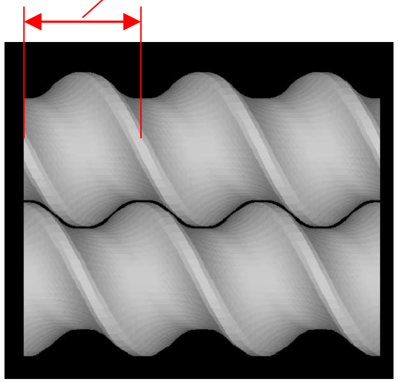
	Barrel radius(mm)		Distance between Axis(mm)		Clearance(mm)
R_b	20.0	C_L	32.85	δ	0.5

Input Parameters

Element Type: Self-wiping screw

(●) Normal ( ) Reverse

Screw radius(mm) R_s	19.5
Tip number	2
Screw pitch(mm)	30
Turns	3

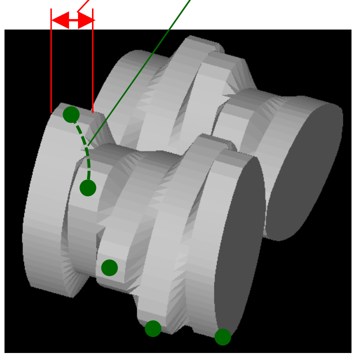


Input Parameters

Element Type: Kneading disc

(●) Normal ( ) Reverse

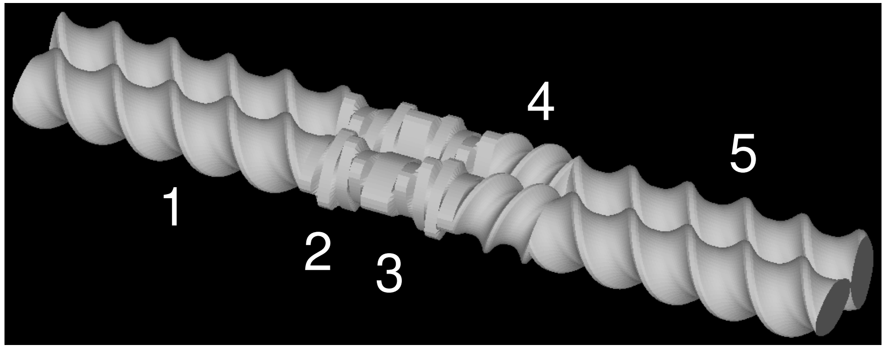
Screw radius(mm) R_s	19.5
Tip number	2
Disk tickness(mm)	8.0
Disk number	5.0
Phase angle	45



Screw Configuration

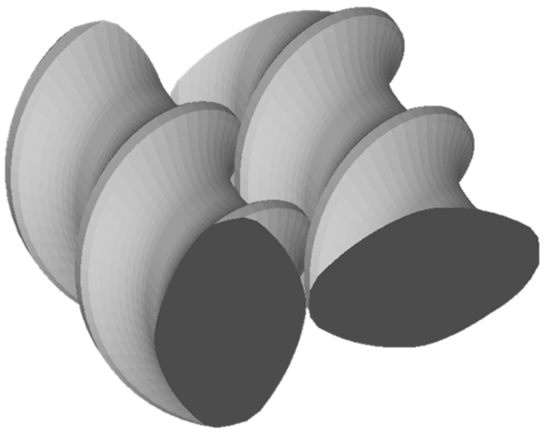
Blk.No.	Type	Rev. or Nor.	Pitch Disk Thick.	Length
1,	SW,	Nor.,	30,	150,
2,	KD,	Nor.,	8.0,	40,
3,	KD,	Rev.,	8.0,	40,
4,	SW,	Rev.,	20,	40,
5,	SW,	Nor.,	30,	150,

Click "Meshing for Visualization"



2.5D FEM Model

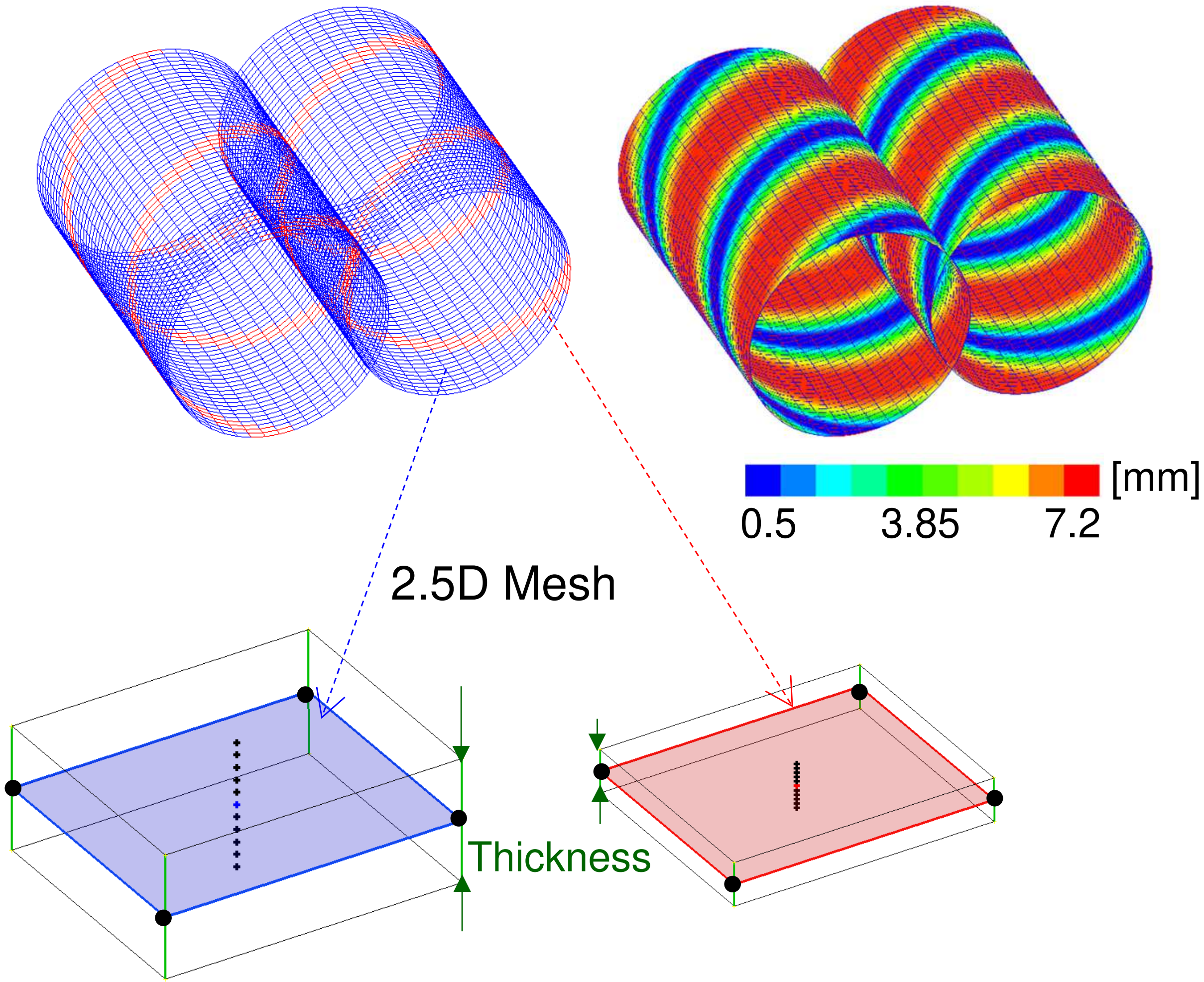
3D Visualized Model



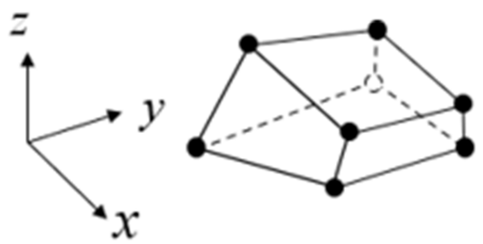
2.5D FEM Model for Analysis

Meshes

Meshes with Thickness



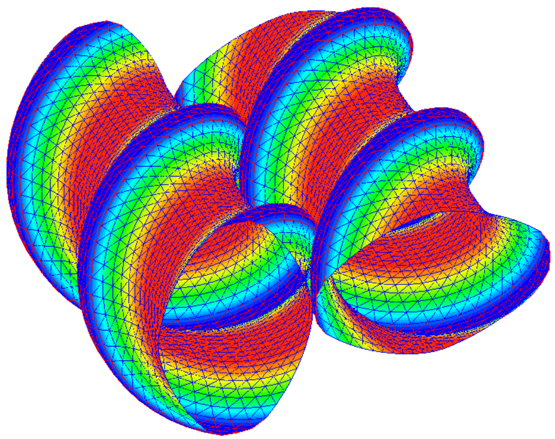
Cf. 3D Mesh



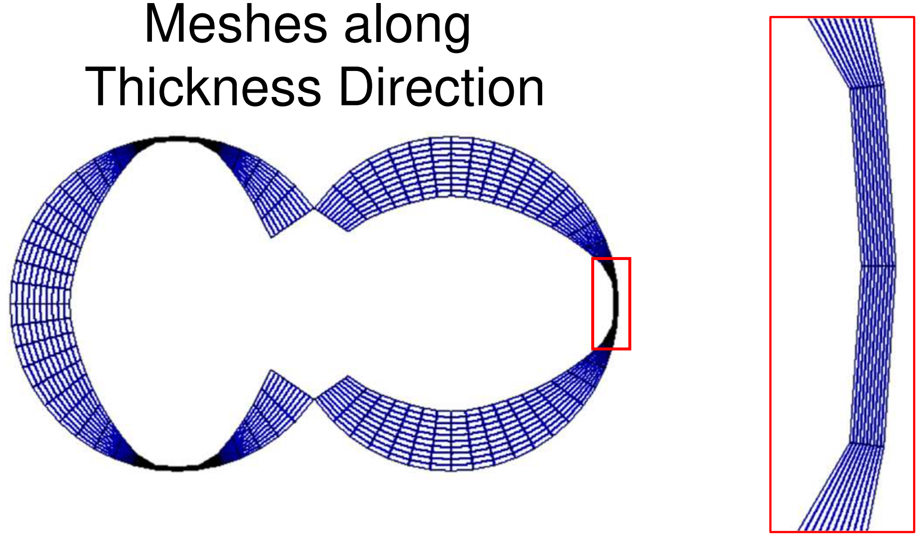
3D Model for Post Process

3D Visualized Model

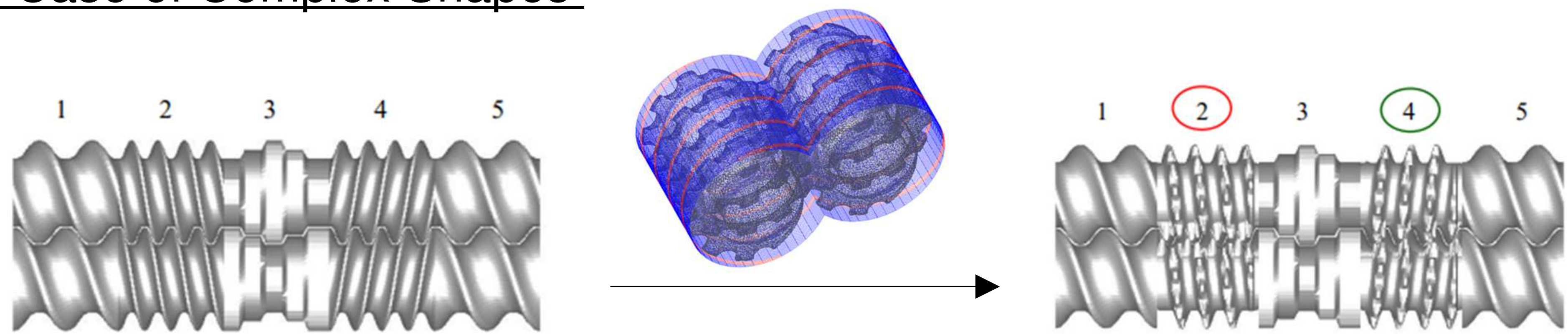
Meshes with Thickness



Meshes along
Thickness Direction



In Case of Complex Shapes



Agenda

1． Twin-Screw Analysis

- 1-1. Development Target
- 1-2. Key Technologies
  1. Modeling
  2. Analyzing
- 1-3. Simulation and Results

2． Multilayer Film Coextrusion Analysis

- 2-1. Key Technologies
- 2-2. Simulation Results

Key Technology 2. Analyzing

Basic Equations on 3D Flow Analysis

- Equation of Motion
- Continuity Equation

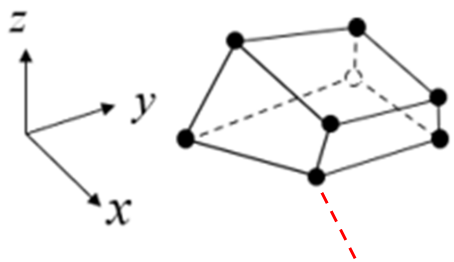
3D FEM (Finite Element Method)

- Discretization by 3D Meshes
- Weak Formulation of the Weighted Residual Method

Flow velocity vector

$$\begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & 0 \end{pmatrix} \begin{pmatrix} u\,(1 \cdots n\max) \\ v\,(1 \cdots n\max) \\ w\,(1 \cdots n\max) \\ p\,(1 \cdots n\max) \end{pmatrix} = \begin{pmatrix} q_u\,(1 \cdots n\max) \\ q_v\,(1 \cdots n\max) \\ q_w\,(1 \cdots n\max) \\ 0\,(1 \cdots n\max) \end{pmatrix}$$

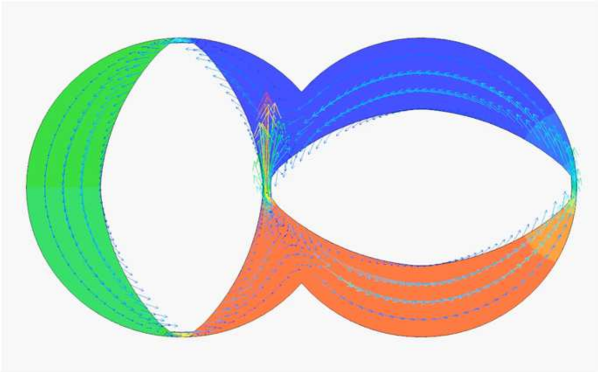
Flow pressure vector

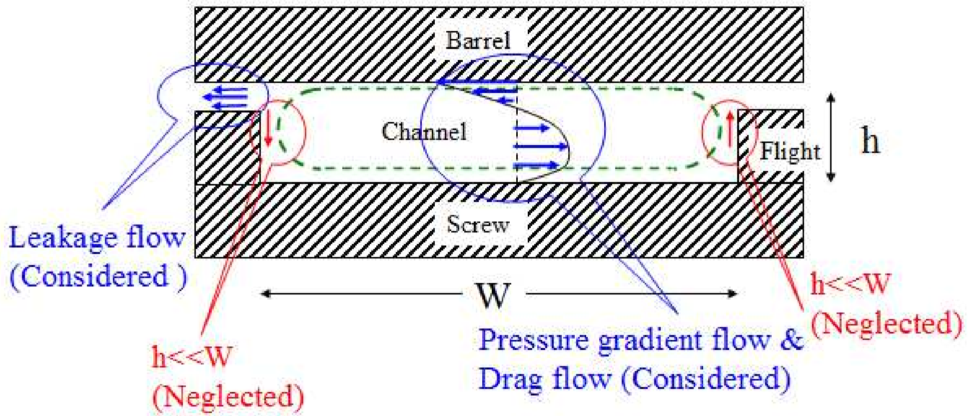


Four Unknows per Node (*u*, *v*, *w*, *p*)

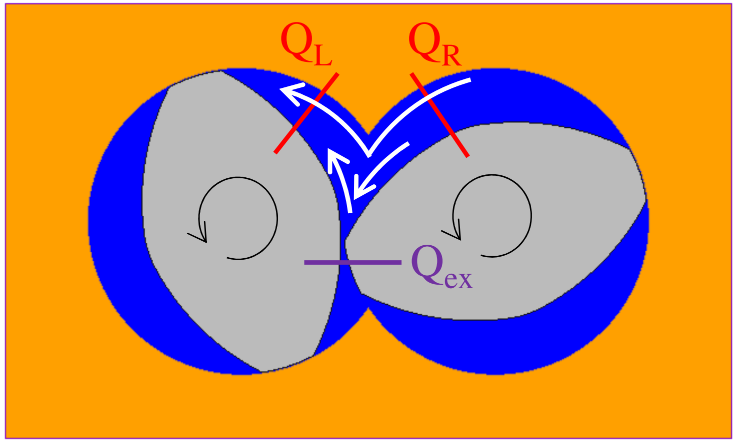
Approximations of Screw Flow for 2.5D FEM

1. Considering Hele-Shaw (Thin-walled) Flow



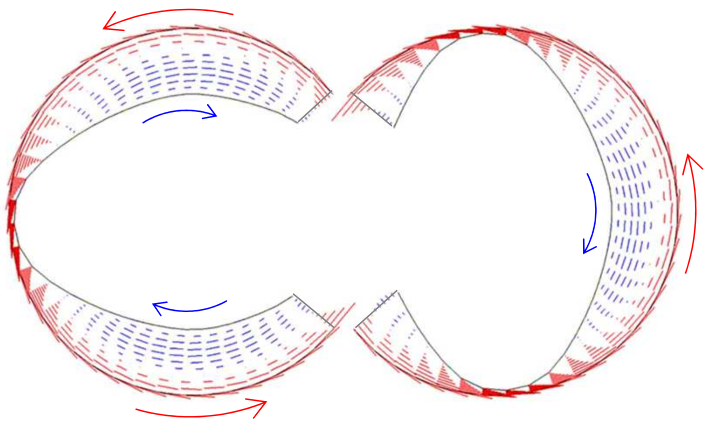


2. Omitting Self Wipe Region



$Q_L = Q_R$

$Q_{ex} \fallingdotseq 0$



2.5D FEM Analysis

Hele-Shaw Flow Approximation

- Substituting Analytical Solution of Equations of Motion into Continuity Equation

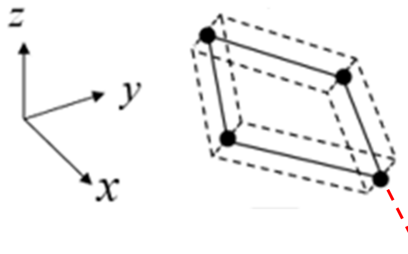
2.5D FEM

- Discretization by 2.5D Meshes
- Weak Formulation of the Weighted Residual Method

$$ {}_{n\max}\left[\times\right]^{n\max}\left(p\left(1\cdots n\max\right)\right)=\left(q\left(1\cdots n\max\right)\right) $$

Pressure

Flow Rate [m^3/sec]



One Unknown per Node (*p*)

Novelty of Developed 2.5D FEM for Screw Flow

Formulation for Injection Molding (since 1970'~)

$$Q_\alpha = S_{\alpha\beta} p_\beta$$

Flow Rate [m³/sec] — Pressure Gradient Flow Rate

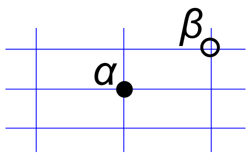
Formulation for Screw Extrusion

$$Q_\alpha = S_{\alpha\beta} p_\beta + D_\alpha$$

Flow Rate [m³/sec] — Drag Flow Rate

α, β : Node Number

$S_{\alpha\beta}$: Flow Conductance

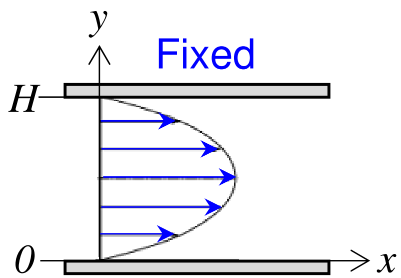


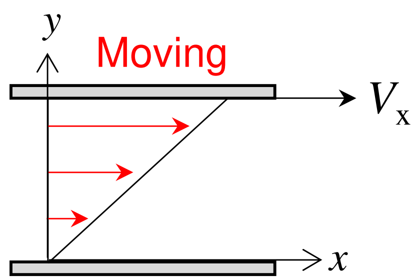
Laminar Flow between Parallel Plates

$$u(y) = \boxed{\frac{y}{2\eta}\left(\frac{\partial P}{\partial x}\right)(y-H)} + \boxed{\frac{V_x}{H} y},$$

η : Viscosity of Polymer Fluid

Velocity [m/sec] — Poiseuille Flow — Couette Flow





Developed Formula for Screw Extrusion

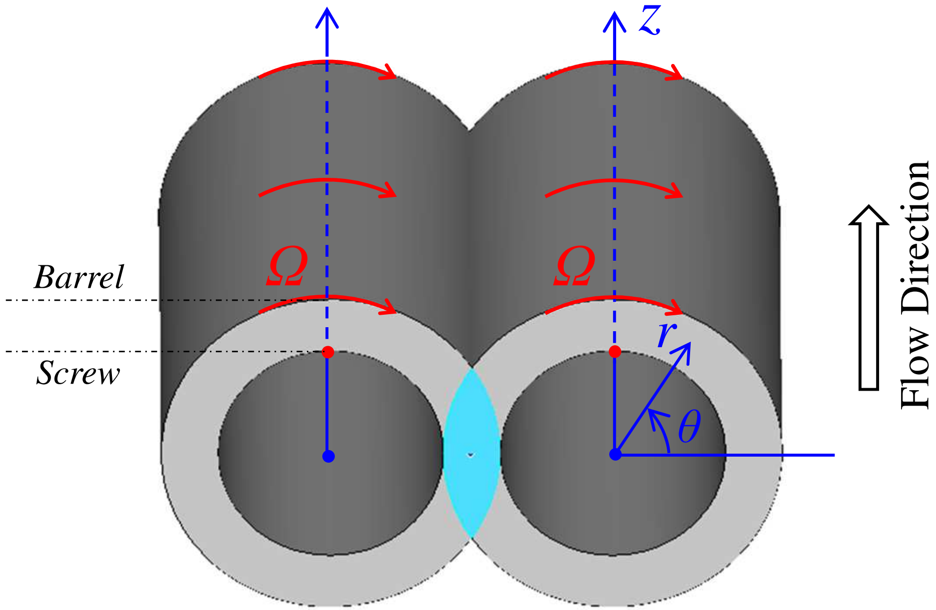
$$Q^{e}_{\alpha} = -\left(S^{e\theta}_{\alpha\beta} + S^{ez}_{\alpha\beta}\right) p^{e}_{\beta} + D^{e}_{\alpha}$$

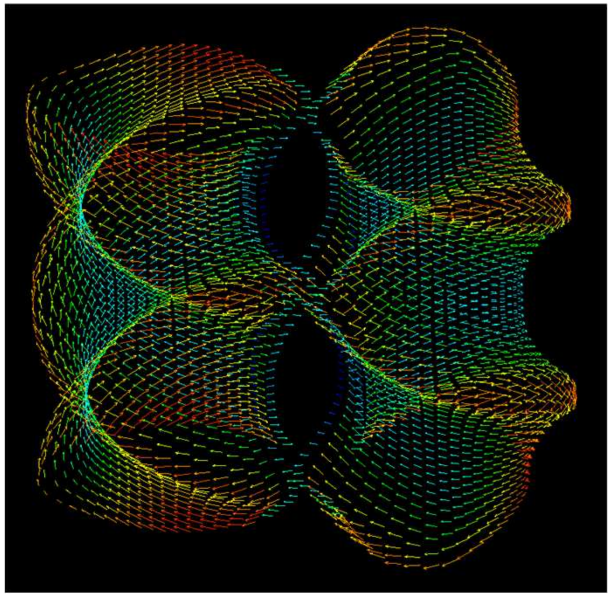
Flow Rate
[m^3/sec]

Pressure Gradient Flow Rate

Drag Flow Rate

Ref.1 in #1056, AIChE J. 2020, *66*, e17018.





Agenda

1． Twin-Screw Analysis

1-1. Development Target

1-2. Key Technologies
    1. Modeling
    2. Analyzing

1-3. Simulation and Results

2． Multilayer Film Coextrusion Analysis

2-1. Key Technologies

2-2. Simulation Results

Simulation Flowchart

Modeling

↓

Input Polymer Properties

Viscosity η , Density,
Thermal Conductivity, Specific Heat

↓

Input Molding Condition

Flow Rate, Screw Rotation Speed,
Barrel Control Temperature

↓

2.5D FEM Analysis

Pressure p,
Velocity, Strain rate,
Temperature
Filling Ratio

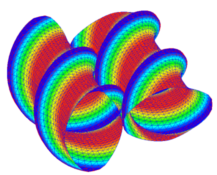
E.g. Velocity along screw length z

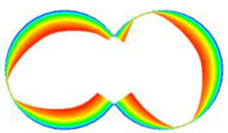
$$v_z(r) = \frac{1}{2}\left(\frac{\partial p}{\partial z}\right)\left(\int_{R_s}^{r} \frac{r}{\eta} dr - \frac{\alpha_c}{\beta_c}\int_{R_s}^{r} \frac{1}{\eta r} dr\right)$$

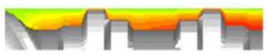
$$\alpha_c = \int_{R_s}^{R_b} \frac{r}{\eta} dr, \quad \beta_c = \int_{R_s}^{R_b} \frac{1}{\eta r} dr$$

↓

Results Visualization

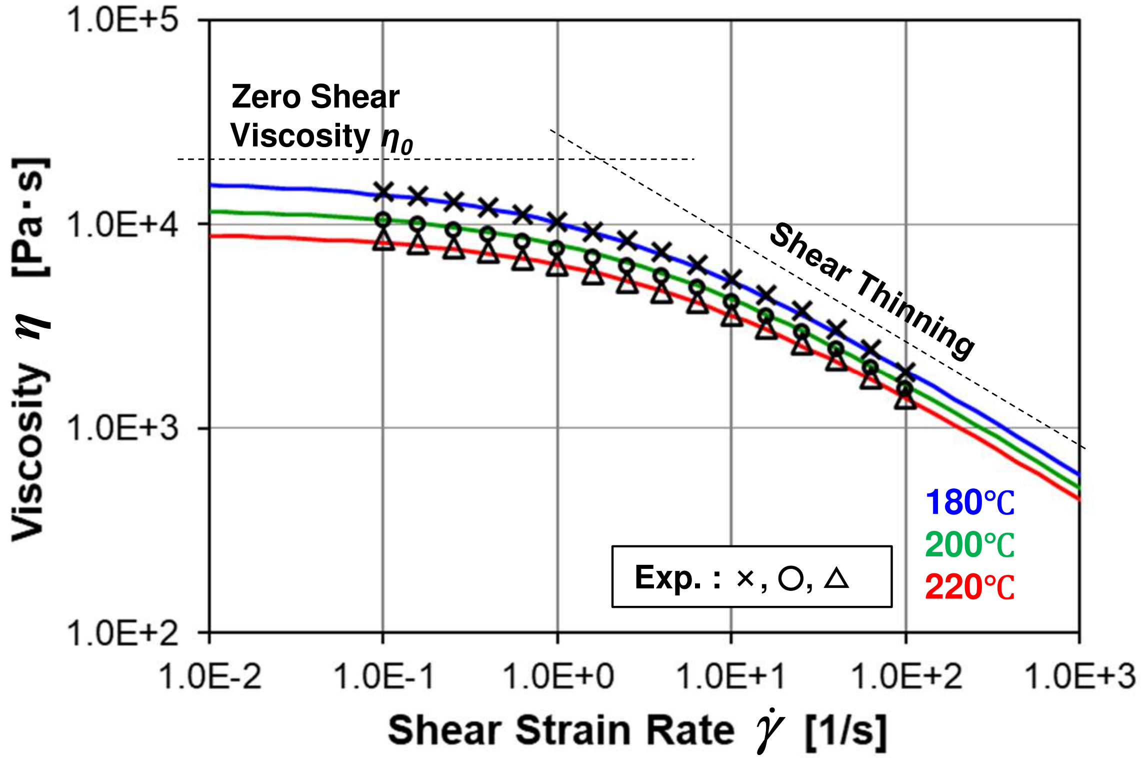




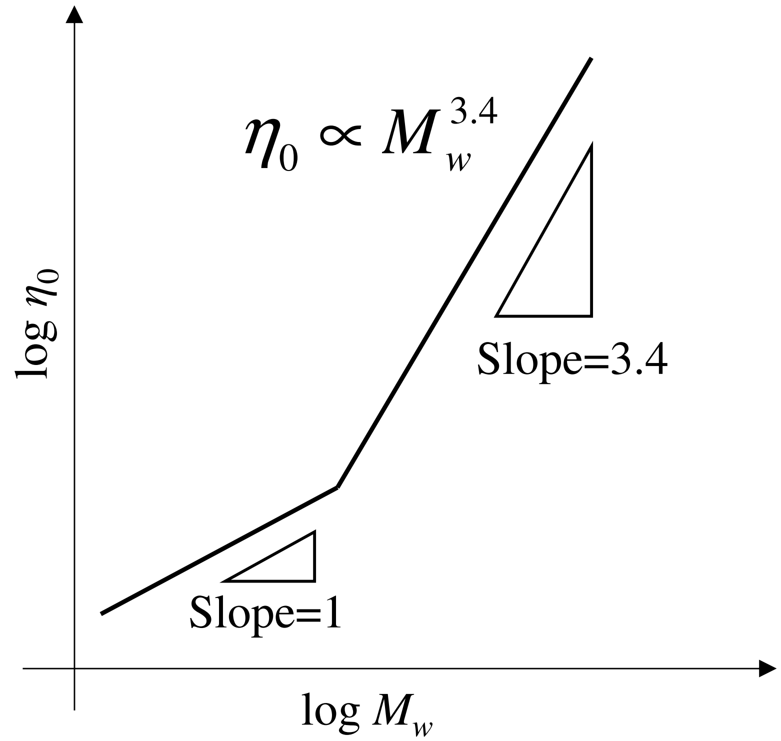


Polymer Viscosity

Flow Curve of HDPE



Relationship between M_w and η_0



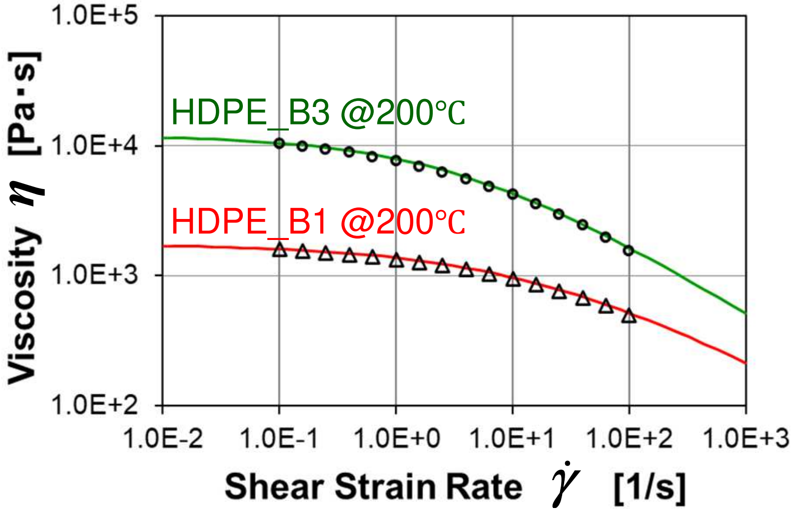
Cross Model

$$\eta = \frac{\eta_0}{1+\left(\eta_0\dot{\gamma}/\tau^*\right)^{1-c}}, \quad \eta_0 = A\exp\left(\frac{T_b}{T+273.15}\right)$$

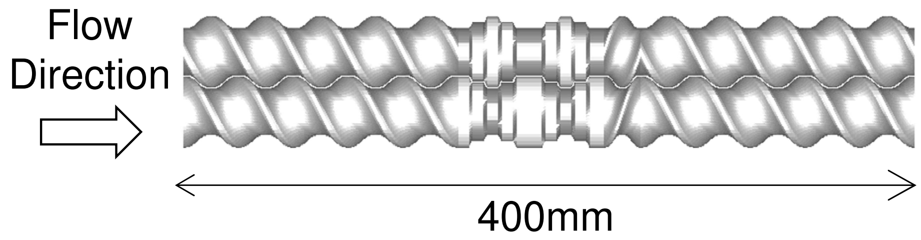
Reference: Fox, T. G. and Flory, P. J.
J. Am. Chem. Soc. ,**70**, 2384-2395(1948)

Effect of Viscosity

Polymer

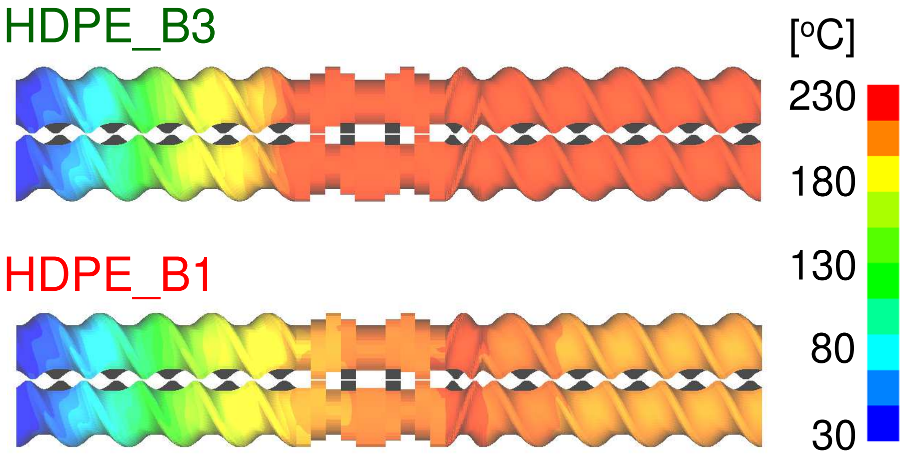


Molding Condition



Mass Flux Rate : 10 kg/h
Screw Rotation Speed : 100 rpm
Barrel Temperature : 200 ℃ max.

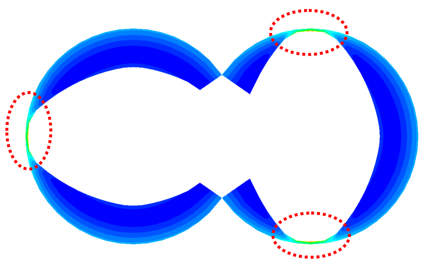
Simulated Temperature



Energy Equation

$$\rho C_p \boldsymbol{u} \nabla T = \kappa \Delta T + \eta \dot{\gamma}^2$$

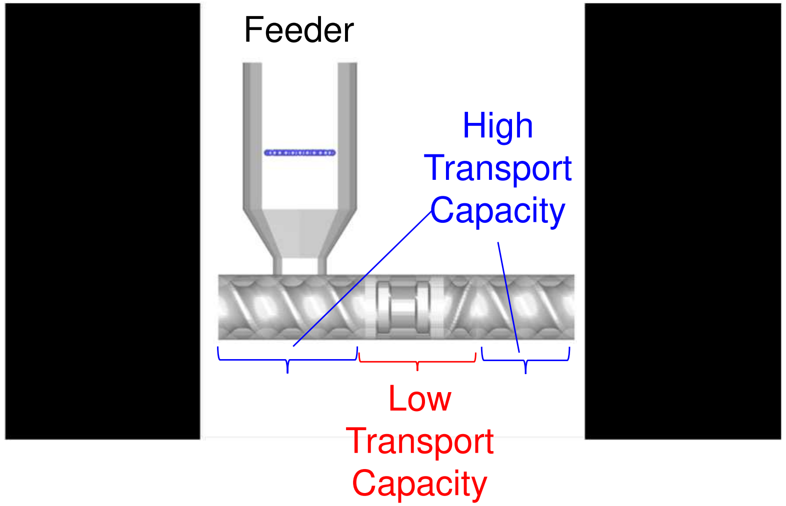
Convection Diffusion Viscous Heat Generation

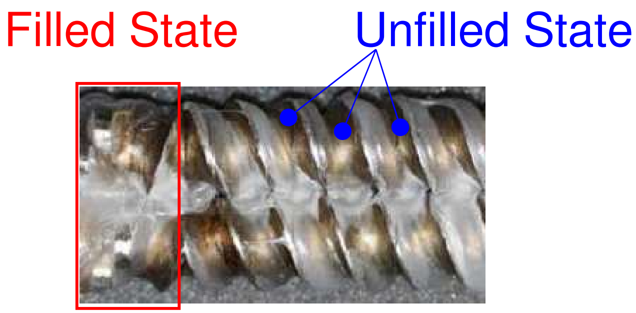


Large $\dot{\gamma}$ value near screw flight

Filling Ratio (Degree of Fill)

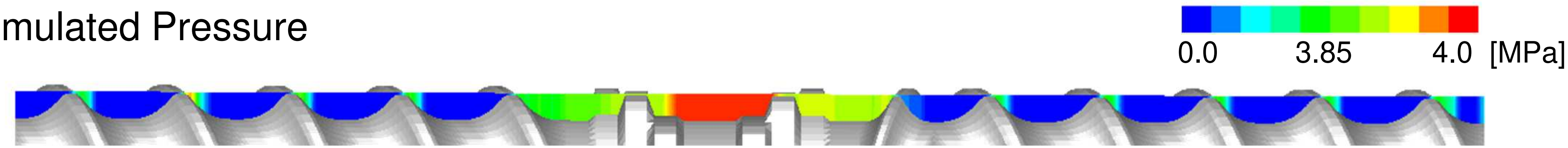
Twin-Screw extruders are operated under starved feeding conditions.



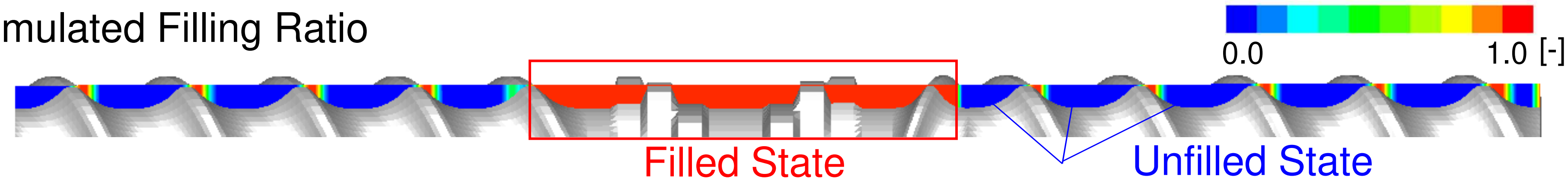


Filling ratio is calculated from balance of flow rate and pressure gradient.

Simulated Pressure



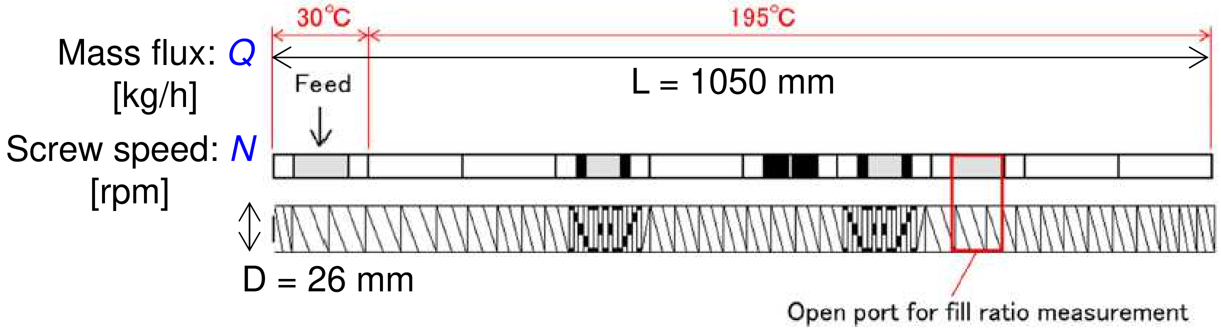
Simulated Filling Ratio

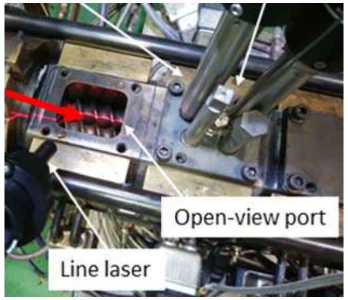


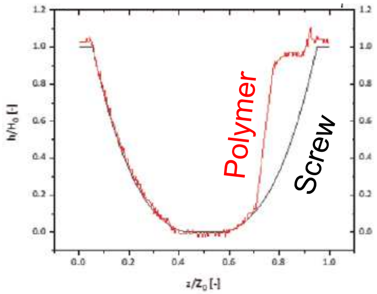
Experimental Verification

Ref.1 in #1056, AIChE J. 2020, *66*, e17018.

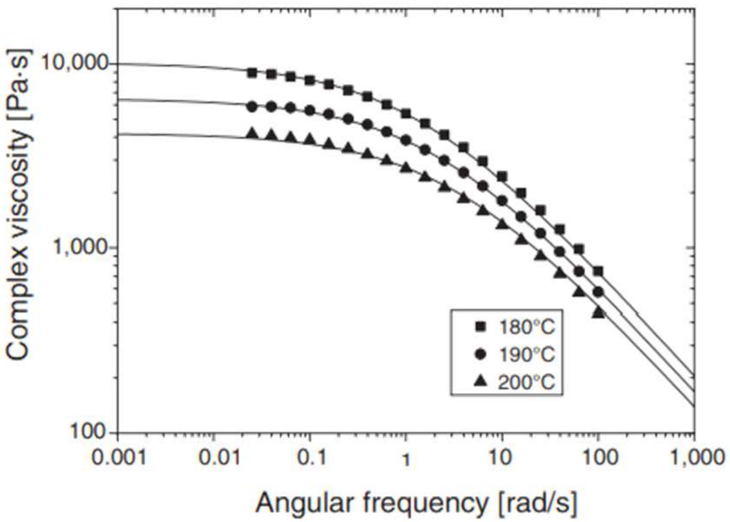
Screw Configuration (Shibaura Machine, Japan)







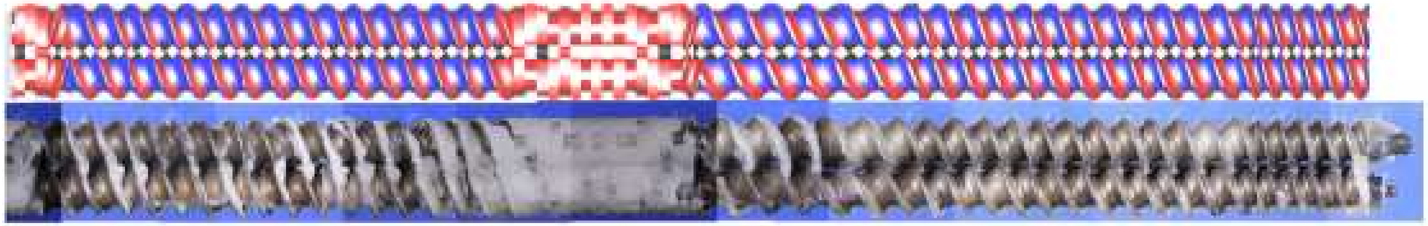
Polymer: Homo Polypropylene (F-704NP, Prime Polymer, Japan)



Experimental Verification: Filling Ratio

Qualitative Comparison by Pull-out Experiment

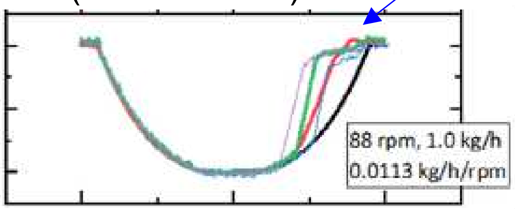
Q: 1.0 kg/h
N: 88 rpm
(Q/N =0.011)



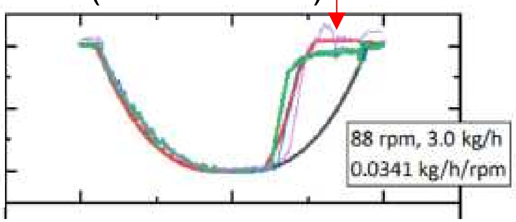
Comparisons under various conditions

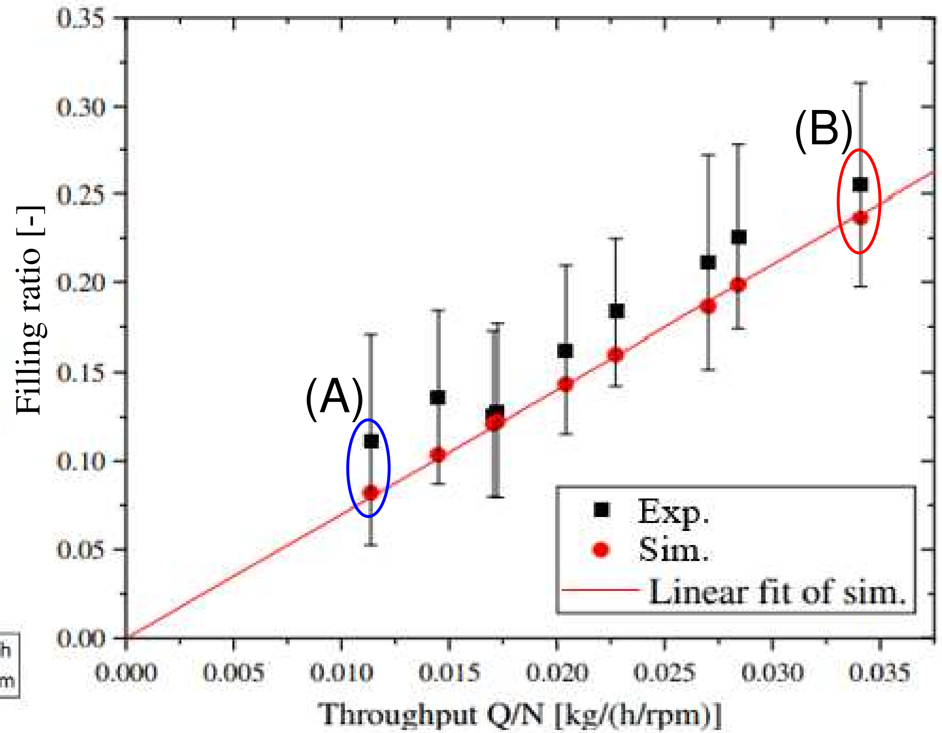
	Screw rotation speed *N*, rpm				
	39	49	58	69	88
Feed rate Q, kg/h 1.0	×	×	×	×	×
1.5	-	-	-	-	×
2.0	-	-	-	-	×
2.5	-	-	-	-	×
3.0	-	-	-	-	×

(A) Q=1.0, N=88
(Q/N =0.011)



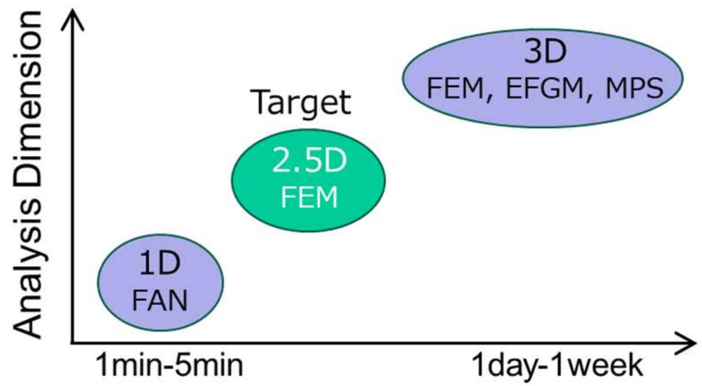
(B) Q=3.0, N=88
(Q/N =0.034)





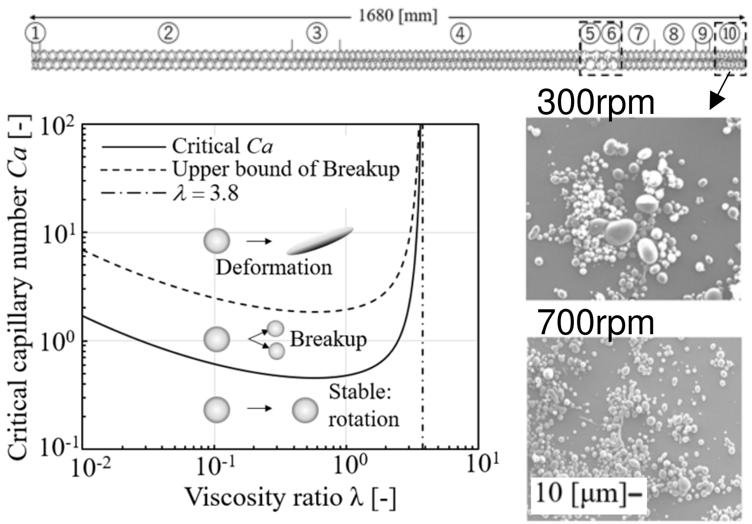
Summary of Twin-Screw Analysis

1. Modeling
   - Numerical Input System
2. Analyzing
   - Overall Screw Length
   - Analysis Time: within One Hour



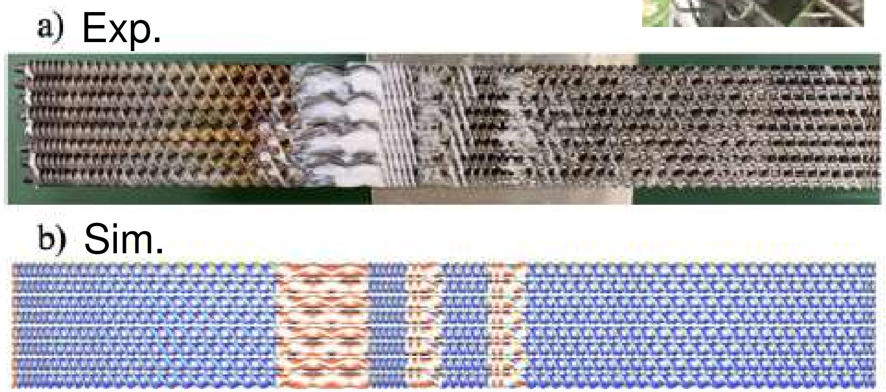
⇒ Recent Efforts

Polymer Blend Morphology



Ref. S. Tanifuji; D. Yorifuji; K. Taki, *J. Soc. Multi. Flow,* 2024, *38*, 139.

Octa-Screw Analysis



Ref. C. Y. Liu; S. Mikoshiba; Y. Kobayashi, A. Ishigami, D. Yorifuji, S. Tanifuji, H. Ito, *Polymer,* 2022, *14*, 1201.

Agenda

1. Twin-Screw Analysis

1-1. Development Target

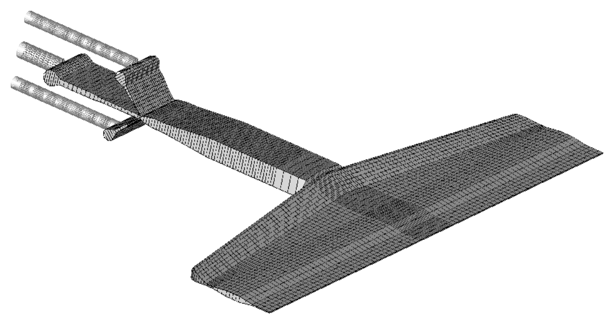
1-2. Key Technologies
   1. Modeling
   2. Analyzing

1-3. Simulation and Results

2. Multilayer Film Coextrusion Analysis

2-1. Key Technologies

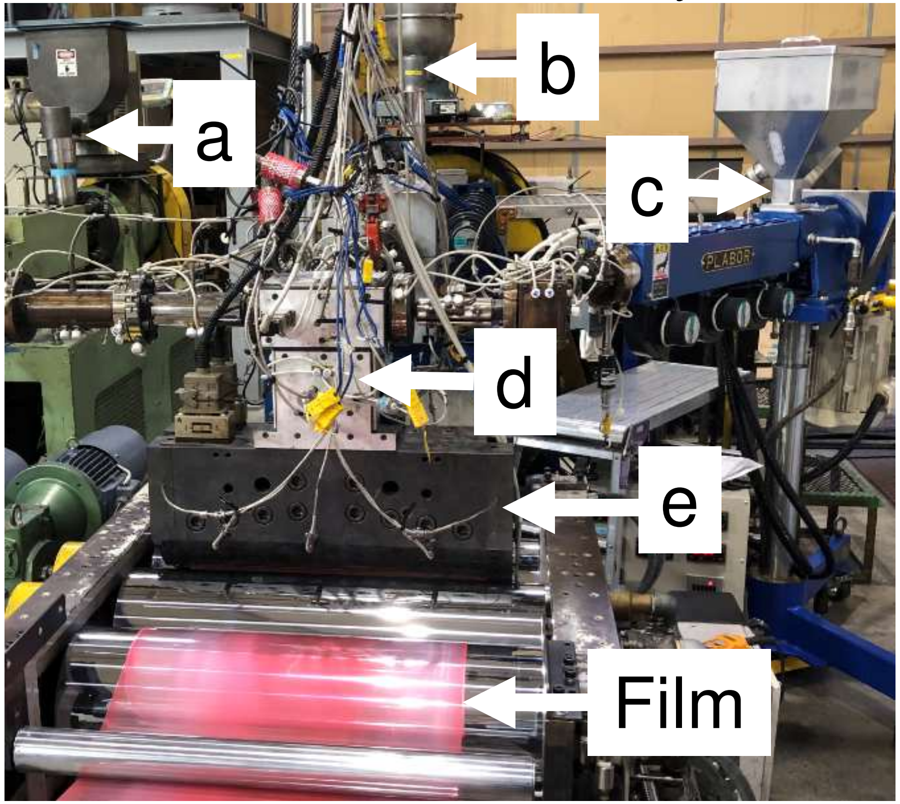
2-2. Simulation and Results



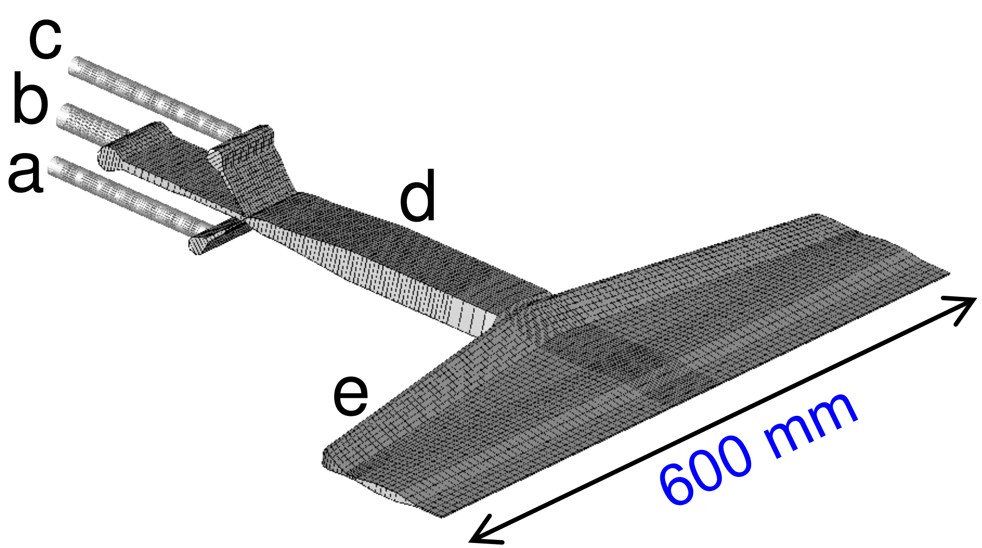
Multilayer Film Coextrusion

(a) Experimental Configuration

a, b, c : extruder of each layer



(b) 3D Visualized Model



d : feedblock

e : flat-die (1mm thick at outlet)

Our 2.5D FEM Scheme

Ref.3 in #1056, Seikei Kakou, 2021, 33,60.

Formulation for Injection Molding (since 1970'~)

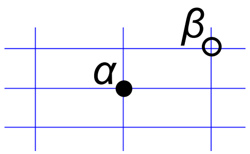
$$Q_\alpha = S_{\alpha\beta} p_\beta$$

Flow Rate [m³/sec]

Pressure Gradient Flow Rate

α, β : Node Number

$S_{\alpha\beta}$: Flow Conductance

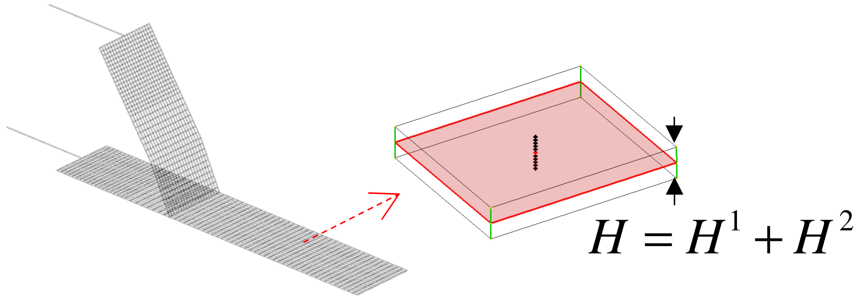


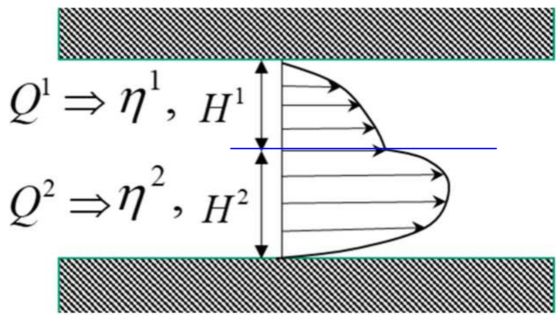
Formulation for Coextrusion Flow

$$Q_\alpha^l = S_{\alpha\beta}^l p_\beta^l + F_\alpha^l$$

$for\ l = 1 \sim n$

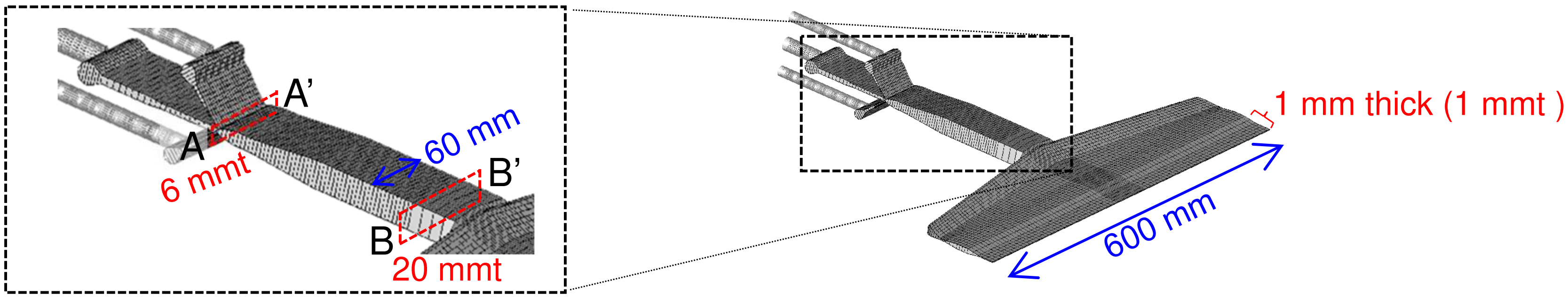
Interaction flow rate with adjacent layers





Problem Considered

"Interfacial Encapsulation" is caused in feedblock with high H/W ratio.

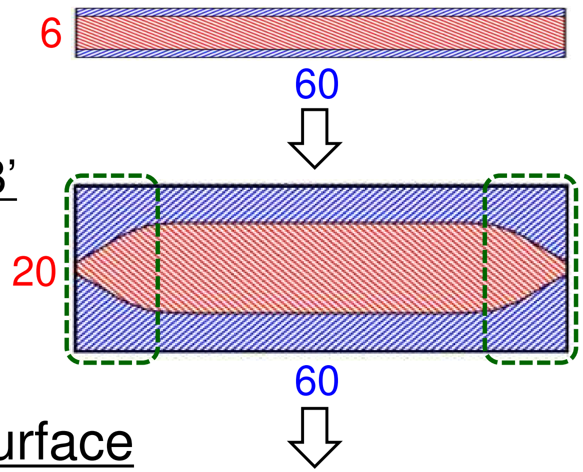


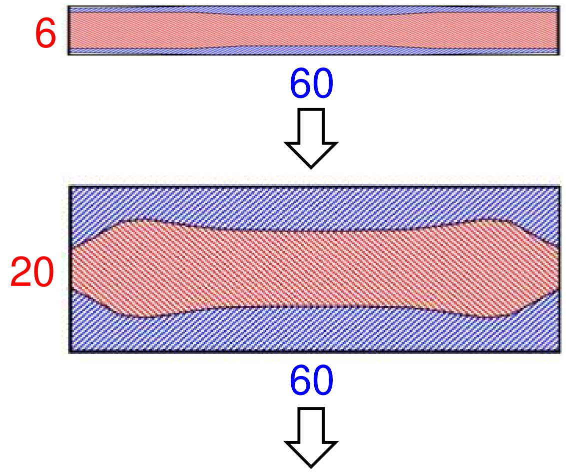
A-A'

a: Flat profile

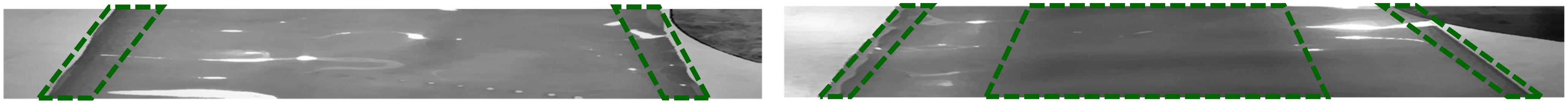
b: Variated profile

B-B'





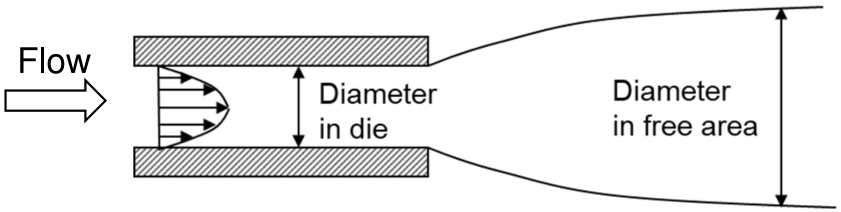
Film surface



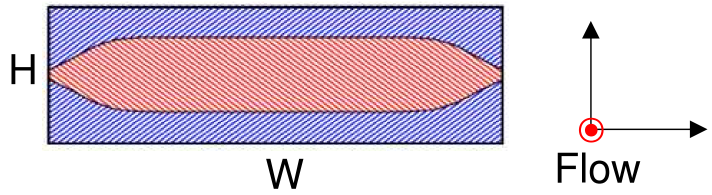
Representation of the encapsulation

"Interfacial Encapsulation" is caused
by the second normal stress difference (N2).

Die Swelling: Effect of N1



Interfacial Encapsulation: Effect of N2



CEF (Criminale Ericksen Filbey) Model for Considering Viscoelastic

Ref. Criminale, Jr. W. O., Ericksen, J. L. and Filbey, Jr. G. L. : Arch. Rat. Mech. Anal., 1, 410 (1985)

$$\tau = 2\eta D - \psi_1 \overset{\nabla}{D} + 4\psi_2 D \bullet D$$

Stress [Pa]	Viscous Stress	Effect of N1	Effect of N2

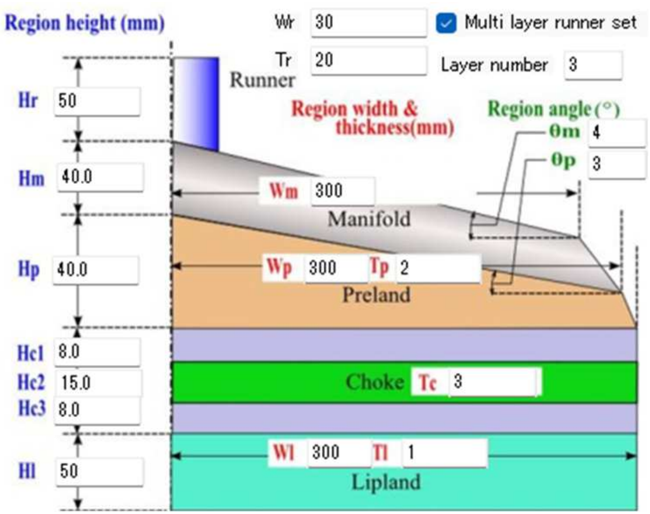
$$D = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) & \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \\ \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) & \frac{\partial v}{\partial y} & \frac{1}{2}\left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right) \\ \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) & \frac{1}{2}\left(\frac{\partial w}{\partial y} + \frac{\partial v}{\partial z}\right) & \frac{\partial w}{\partial z} \end{bmatrix}$$

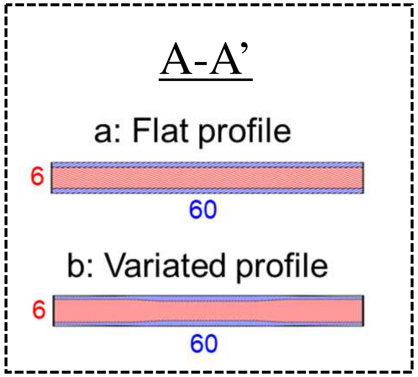
Experimental Verification

Ref.4 in #1056, Seikei Kakou, 2021, *33*, 447.

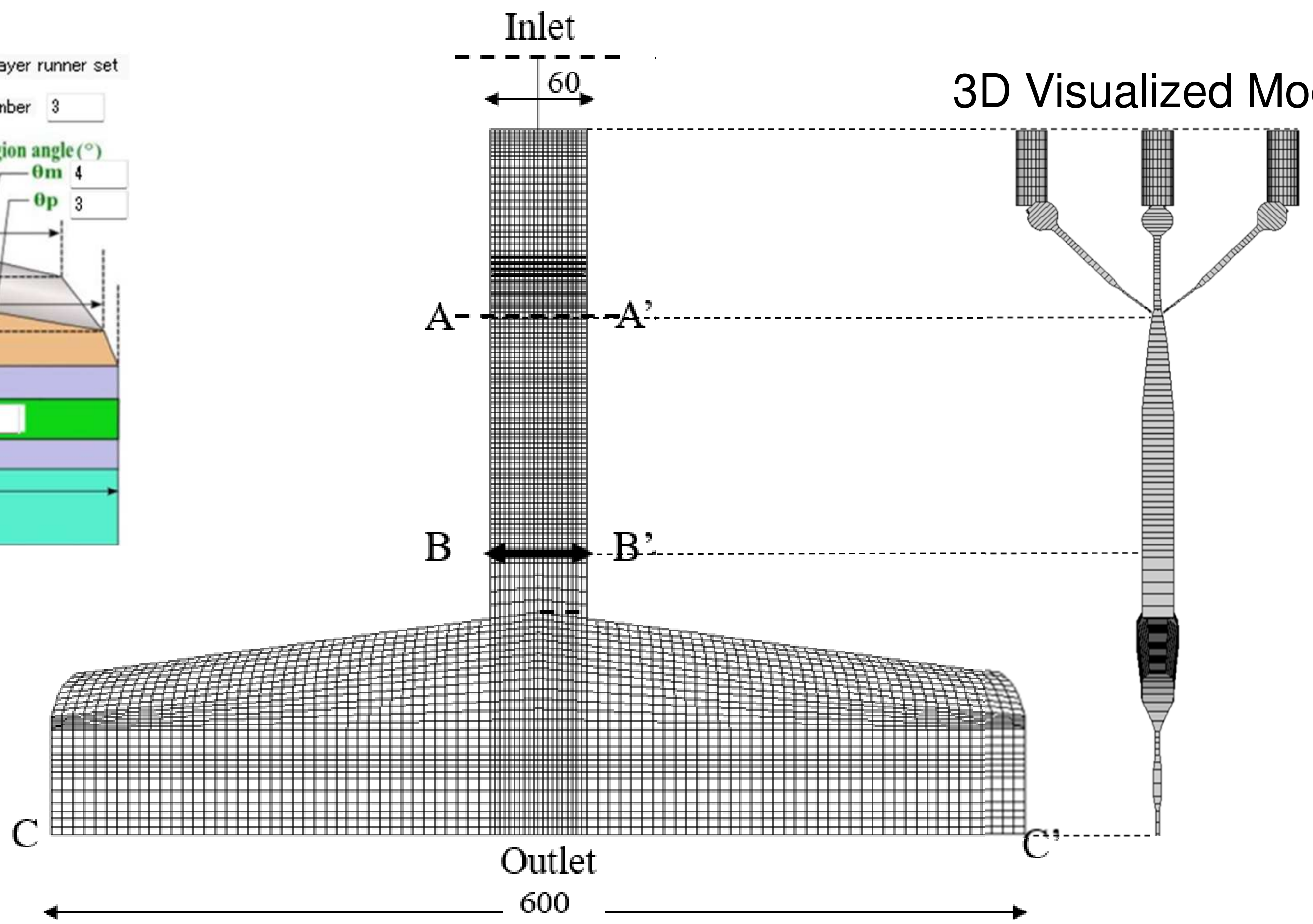
2.5D Model for Analysis

GUI Form





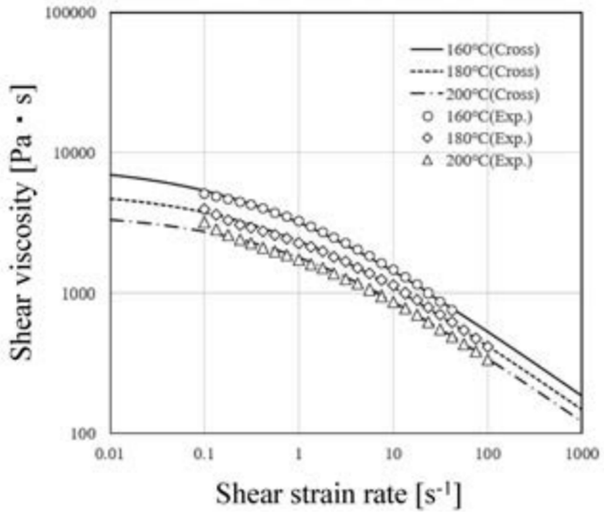
3D Visualized Model



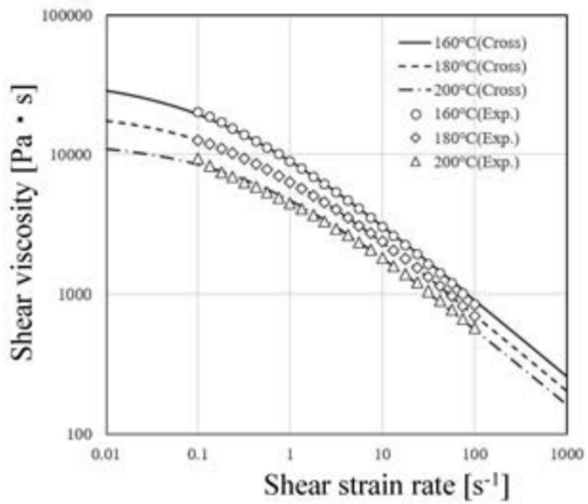
Experimental Verification

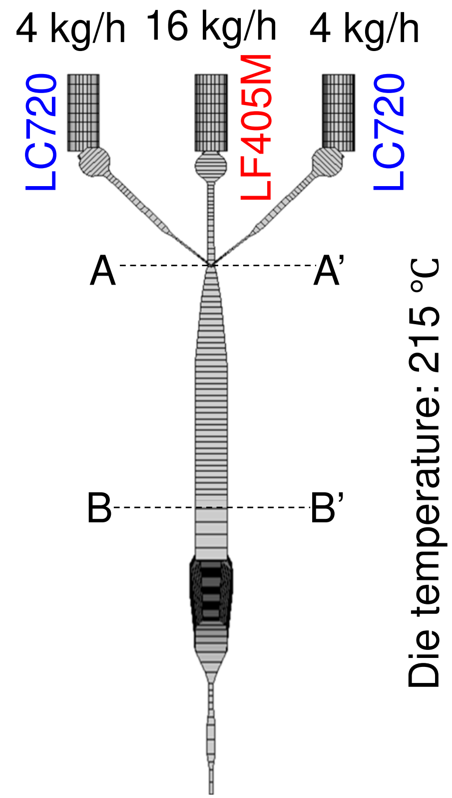
Polymer: LDPE (Japan Polyethylene)

LC720



LF405M



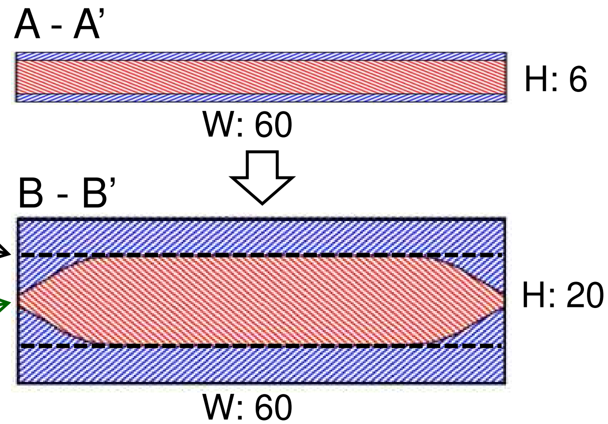


ψ_2 for N2:

Case	Second normal stress difference coefficient : ψ_2[Pa・s²]		
	LC720	LF405M	LC720
0	0	0	0
1	0	−60	0
2	−8	−60	−8
3	−10	−60	−10
4	−18	−60	−18

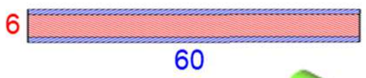
Pure viscosity

Viscoelasticity

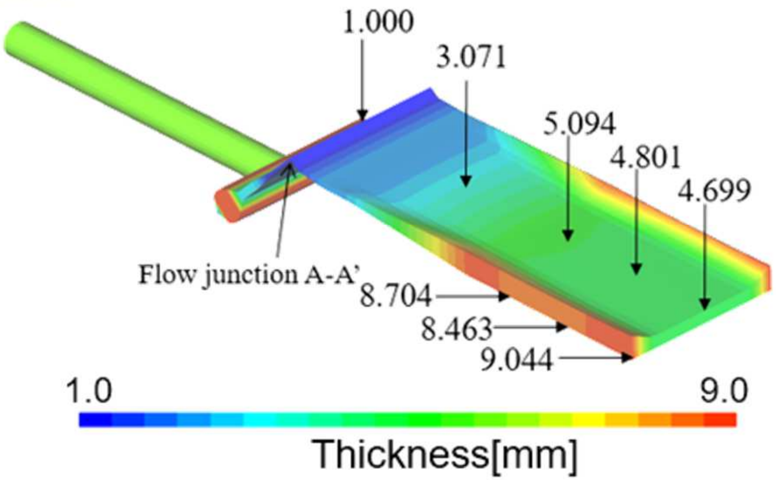


Results of Feedblock

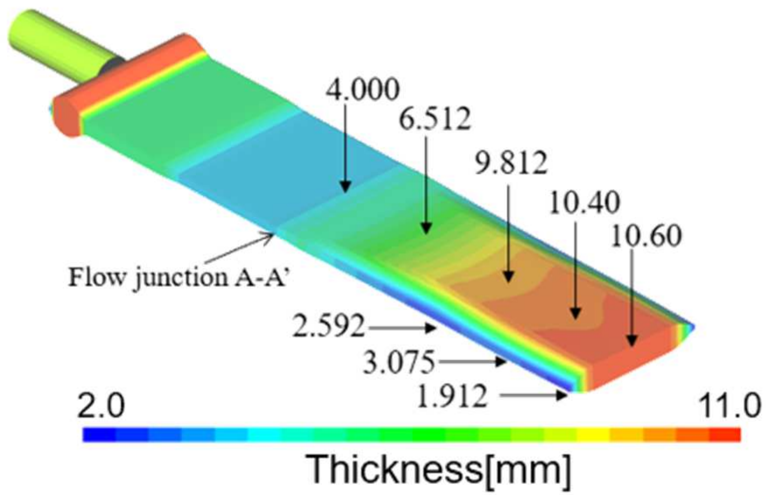
a: Flat profile



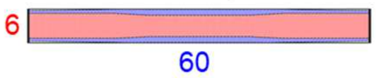
Surface layer: LC720



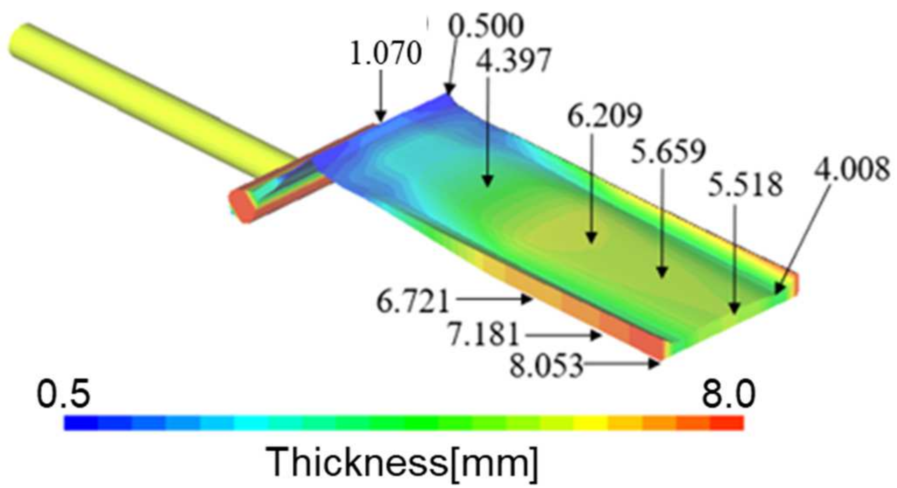
Middle layer: LF405M



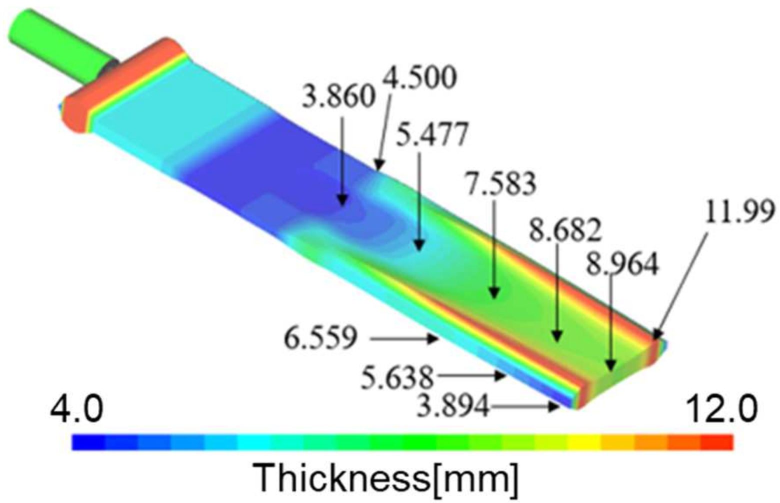
b: Variated profile



Surface layer: LC720

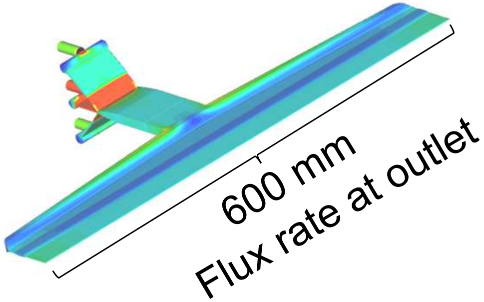


Middle layer: LF405M

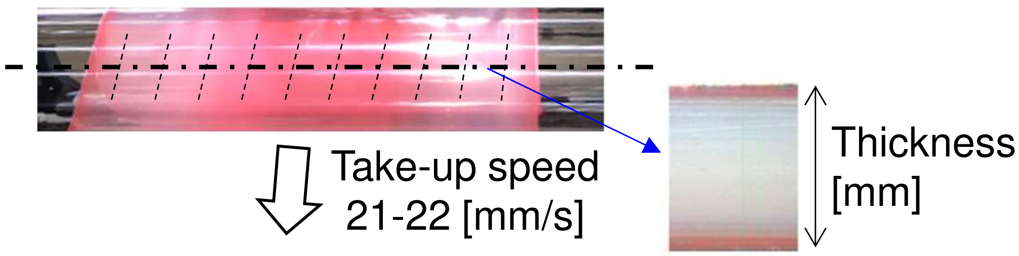


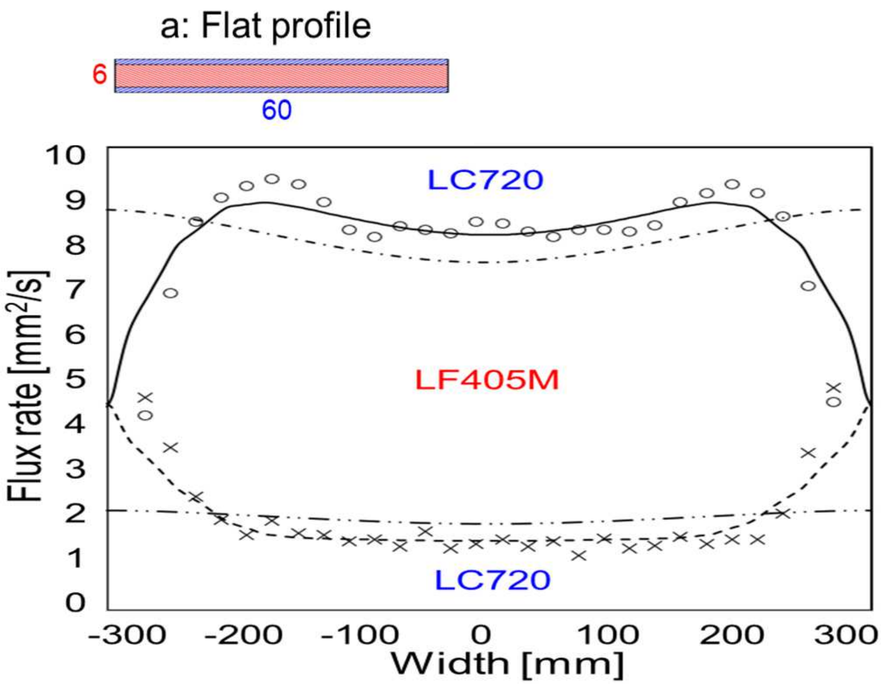
Results of Flat-Die

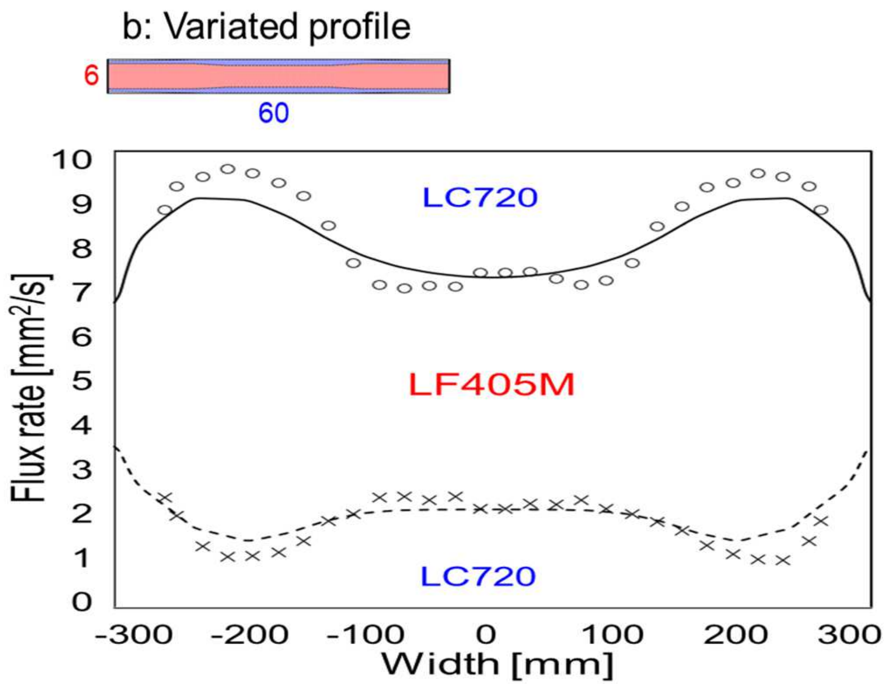
Sim. : Solid and Broken line



Exp. : O and ×





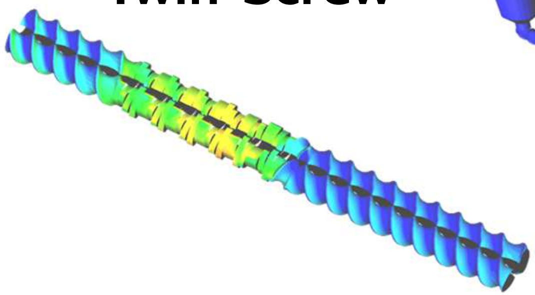


Conclusion

Practical Thermal Flow Analysis on Extrusion Molding
Using 2.5D Finite Element Method

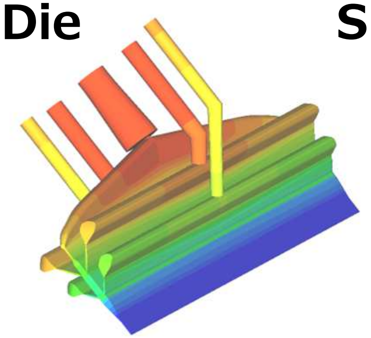
- We developed a novel 2.5D FEM technology on extrusion molding.
- Effectiveness was demonstrated by experimental verifications.
- Calculation time was within an hour under any conditions as shown here.
- Thus we believe that our CAE software is a practical tool for predicting molding conditions in real molding plants.

Twin-Screw

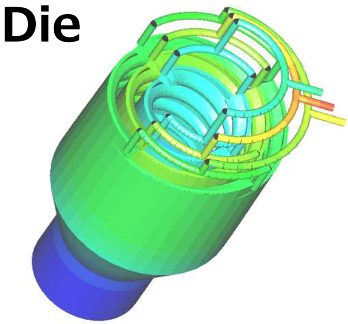


Single-Screw

Flat-Die



Spiral Die



Acknowledgement

References

1. M. Ohara; S. Tanifuji; Y. Sasai; T. Sugiyama; S. Umemoto; J. Murata; I. Tsujimura; S. Kihara; K. Taki, *AIChE J.* 2020, *66*, e17018.

2. M. Ohara; Y. Sasai; S. Umemoto; Y. Obata; T. Sugiyama; S. Tanifuji; S. Kihara; K. Taki, *Polymers,* 2020, *12*, 2728.

3. S. Tanifuji; D. Yorifuji; T. Kibou; M. Tatsumi, *Seikei Kakou*, 2021, *33*, 60.

4. S. Tanifuji; D. Yorifuji; T. Kibou; M. Tatsumi, *Seikei Kakou*, 2021, *33*, 447.

Thank You for Your Attention.

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URL:https://www.hasl.co.jp