押出成形 CAE における
新規 2.5D FEM 解析技術の活用と今後の展望

Applications of new 2.5D FEM Analysis Technology in Extrusion CAE and Future Prospections

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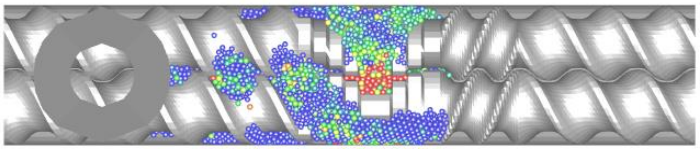
HASL Hyper Advanced Simulation Laboratory

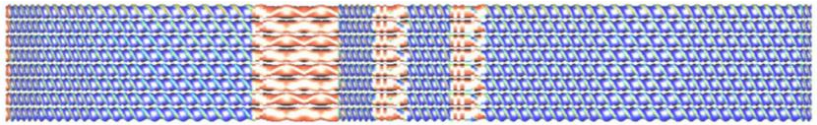
☐ Purpose

Practical 2.5D FEM simulation for polymer extrusion process

Single screw

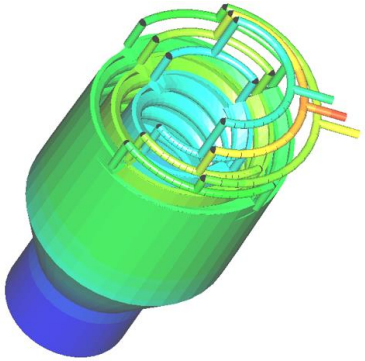


Twin screw

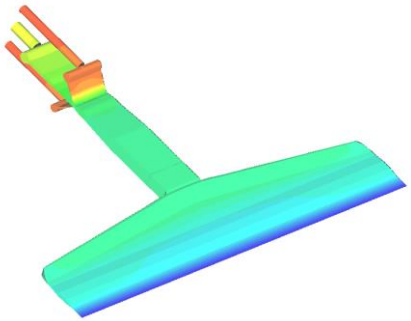


Octa screw

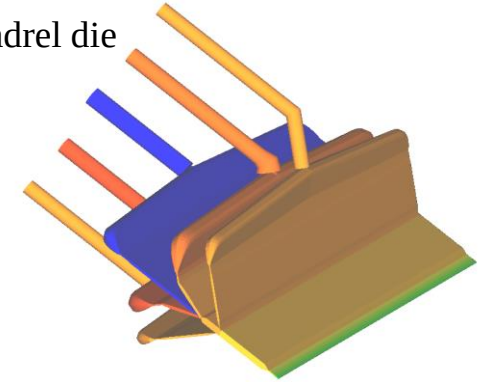
Screw extruder



Multi layer spiral mandrel die



Feed block type multi die



Multi manifold die

Extrusion die

Fig. 1 Various equipments used in the extrusion molding

☐ Recently published papers concerning 2.5D FEM

1) Ohara, M., Tanifuji, S., Sasai, Y., Sugiyama, T., Umemoto, S., Murata, J., Tsujimura, I., Kihara, S. and Taki, K.
「Resin Distribution along Axial and Circumferential Directions of Self-Wiping Co-Rotating Parallel Twin-Screw Extruder」
AIChE J.,**66**,11,e17018(2020)
Twin Screw

2) Ohara, M., Sasai, Y., Umemoto, S., Tanifuji, S., Kihara, S. and Taki, K.
「Experimental and Numerical Simulation Study of Devolatilization in a Self-Wiping Corotating Parallel Twin-Screw Extruder」
Polymers, **12**,11,2728(2020)
Twin Screw

3) Tanifuji, S., Yorifuji, D., Kibou, T. and Tatsumi, M.
「A Generalized 2.5D FEM Formulation for Steady Non-Newtonian Viscous Multi Flow Part 1: Formulation and Theoretical Verification」
Seikei-Kakou, **33**,2,60(2021)
Multi Layer Die

4) Tanifuji, S., Yorifuji, D., Kibou, T. and Tatsumi, M.
「A Generalized 2.5D FEM Formulation for Steady Non-Newtonian Viscous Multi Flow Part 2: Implementation of Pseudo Encapsulation Model and Experimental Verification」
Seikei-Kakou, **33**,12,447(2021)
Multi Layer Die

5) Liu, C., Mikoshiba, S., Kobayashi, Y., Ishigami, A., Yorifuji, D., Tanifuji, S. and Ito, H.
「Experimental Investigation and Numerical Simulation of a Self-Wiping Corotating Parallel Octa-Screw Extruder」
Polymers, **14**,6,1201(2022)
Octa Screw

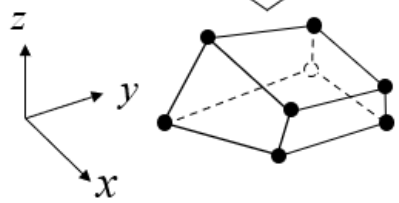
☐ Back ground of 2.5D FEM formulation

3D FEM

Stokes equation (Parabolic type)

Continuity equation (Incompressible)

Discretization



Method of Weighted Residuals

Weak form $\begin{pmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & 0 \end{pmatrix} \begin{pmatrix} u \\ v \\ w \\ p \end{pmatrix} = \begin{pmatrix} \times \\ \times \\ \times \\ \times \end{pmatrix}$ solved by direct matrix solver

2.5D FEM

Stokes equation (Parabolic type)

Semi analytical integration

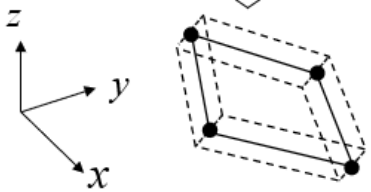
Semi analytical solution

Continuity equation (Incompressible)

Averaging in thickness direction

Pressure equation (Elliptic type)

Discretization



Method of Weighted Residuals

Weak form $(\times)(p)=(\times)$ solved by iterative matrix solver

(u, v, w) : Flow velocity vector

p : Flow pressure

Fig. 2 Comparison of 3D and 2.5D FEM discretization procedures

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Generalization of 2.5D FEM formulation

Pressure equation

Original Form since 1970'~ (Cornell university)

Flow analysis in injection molding
Flow analysis in mono layer extrusion die

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

Q_α: Flux
$S_{\alpha\beta} p_\beta$: Pressure gradient flow

Generalization
in semi analytical integration

Generalized Form

Flow analysis in screw extruder

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

D_α: Drag flow

Flow analysis in multi layer extrusion die

$$Q_\alpha^l = S_{\alpha\beta}^l p_\beta^l + F_\alpha^l = 0 \quad for\ l = 1 \sim n$$

F_α^l: Interaction flow with adjacent layers

α, β : Nodal number
$S_{\alpha\beta}$: Flow conductance matrix D_α, F_α^l : Load vector

Fig. 3 Generalized form of the pressure equation

Free (Layer) surface tracking method

Multi purpose method

Eulerian method :

- VOF
- Level-Set
- CIP

Arbitrary Lagrangian Eulerian method :

- ALE

Particle method :

- DEM
- SPH
- MPS

Free surface updated by using
flow velocity vector information

Problem oriented method in 2.5D FEM

Un-fill state in screw extruder :

Rearrangement of the pressure distribution

$$p(\theta,z)=p(\theta+\Delta\theta,z+\Delta z)-\frac{\partial p}{\partial\theta}\Delta\theta-\frac{\partial p}{\partial z}\Delta z$$

Multi layer surface :

Balance equation of the normal stress on multi layer surface

$$-p^{I}+2\eta^{I}\frac{1}{h^{I}}\frac{Dh^{I}}{Dt}=-p^{II}+2\eta^{II}\frac{1}{h^{II}}\frac{Dh^{II}}{Dt}$$

Free surface updated by using
flow pressure information

Fig. 4 Various free surface tracking methods

☐ Application for the twin screw extruder

「Resin Distribution along Axial and Circumferential Directions of Self-Wiping Co-Rotating Parallel Twin-Screw Extruder」[1)]

Experimental information

Numerical prediction

Transport direction

Homo polypropylene (F-704NP)
supplied by Prime Polymer (Japan)

Fig.5 Qualitative comparison of the resin fill distribution measured during the experiment and predicted by the simulation for 1 kg/h and 88 rpm

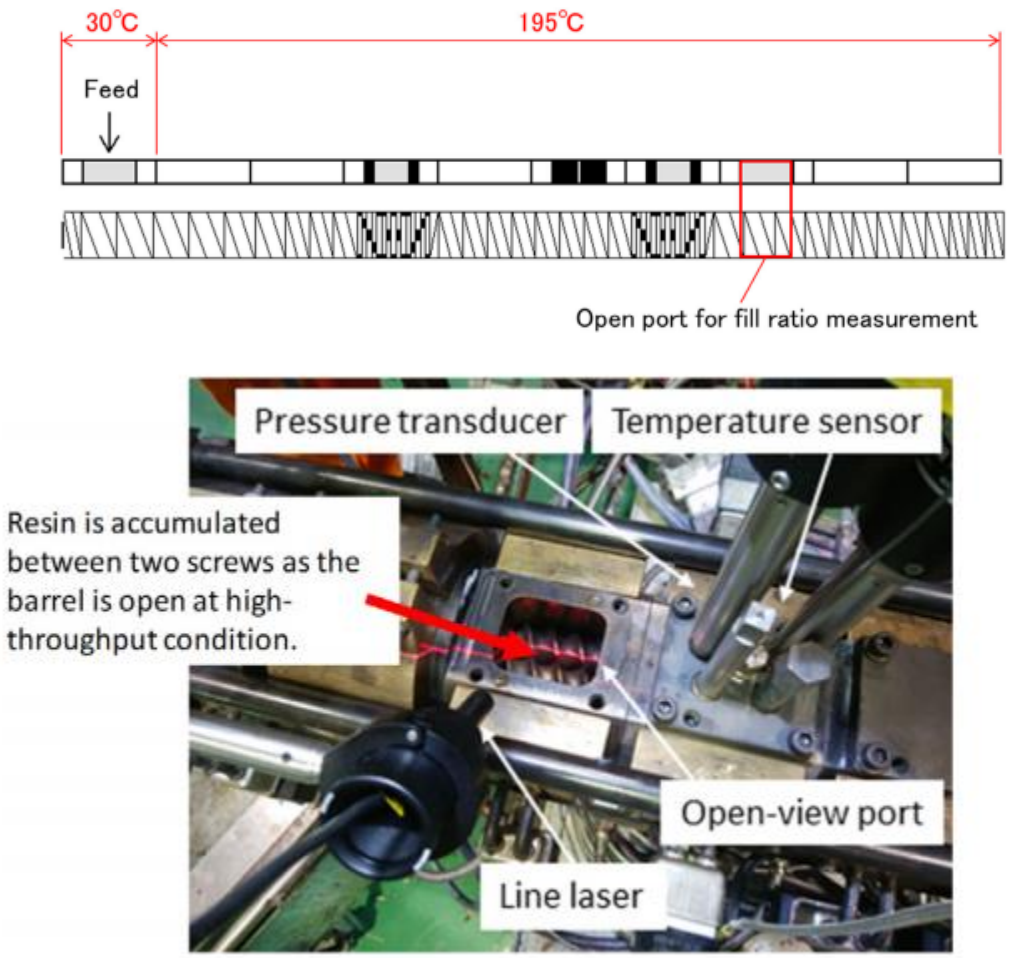
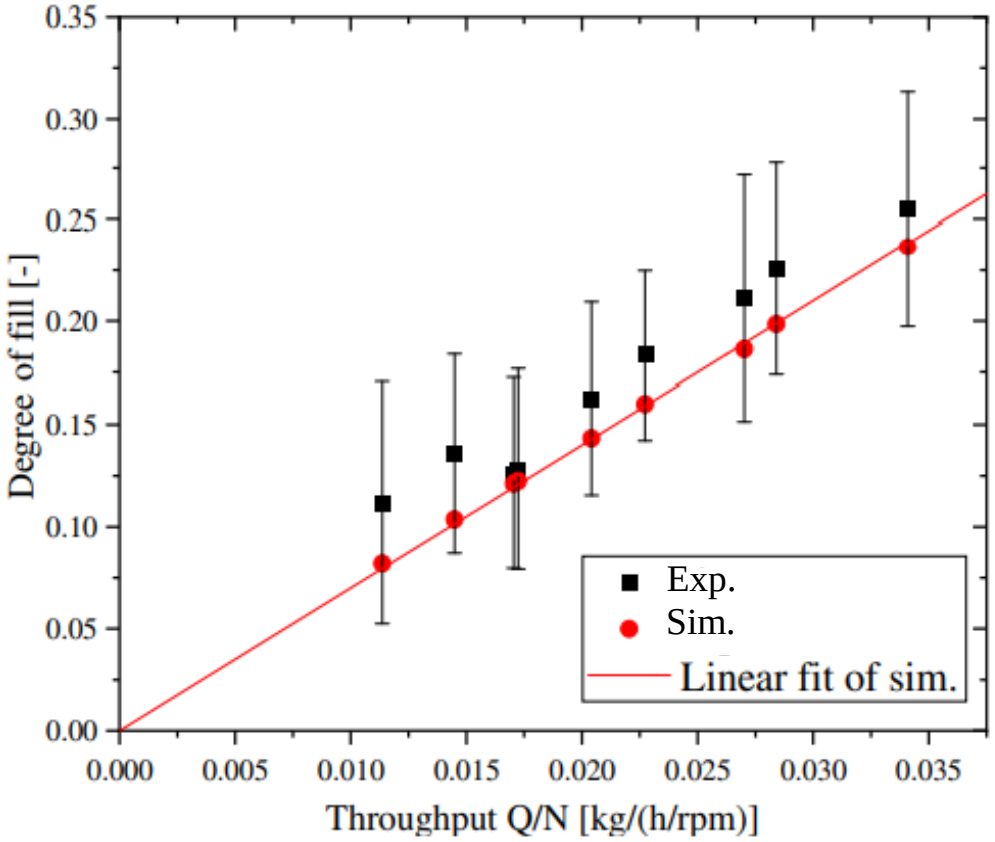


Fig.6 Open-view port of TSE and line laser



Theoretically

$$f = \frac{Q}{Q_d} = \frac{1}{g}\frac{Q}{N}$$

Fig.7 Comparison of simulation and experimental results for the effect of throughput on the degree of fill

「Experimental and Numerical Simulation Study of Devolatilization in a Self-Wiping Corotating Parallel Twin-Screw Extruder」[2)]

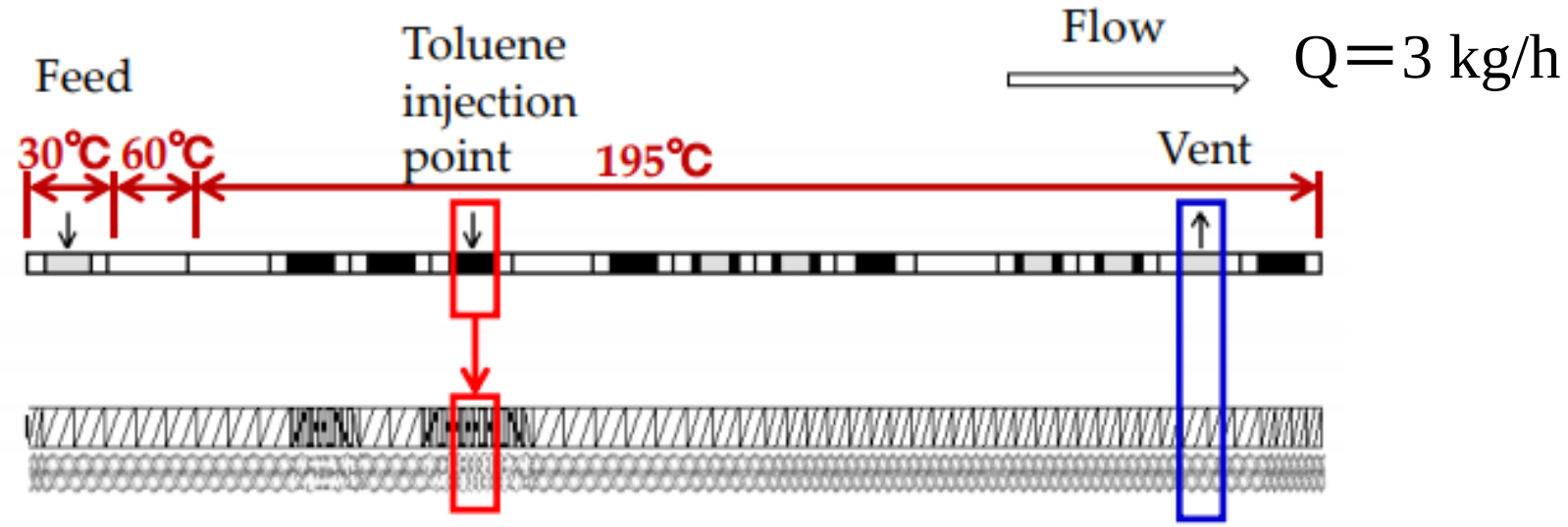
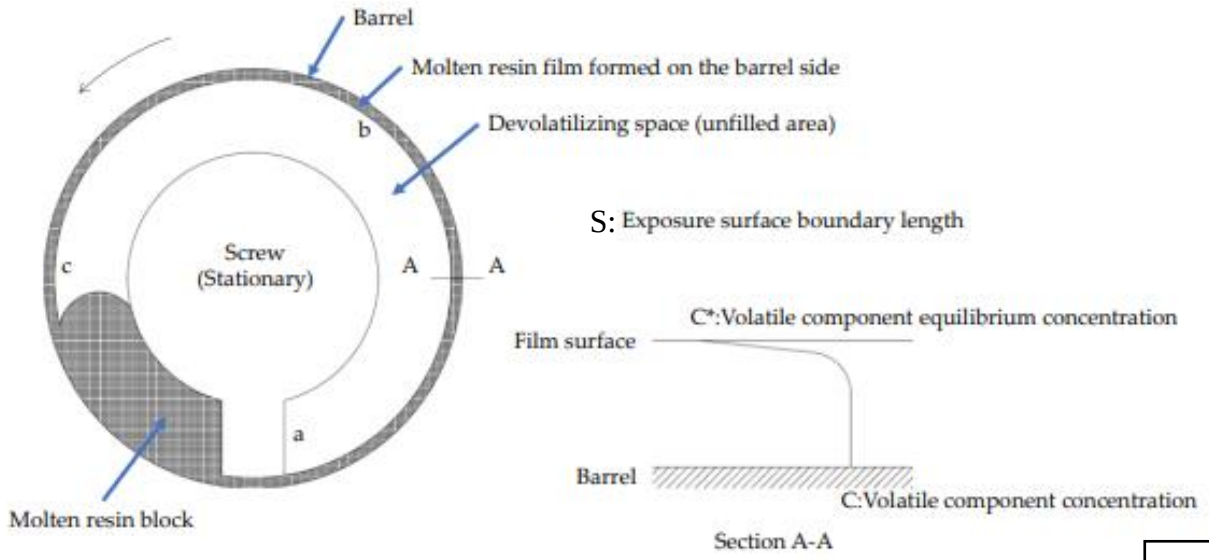


Fig.8 Screw configuration and barrel temperature settings



$$\chi = \frac{C(z_s) - C^*}{C(z_e) - C^*} = \exp\left(\frac{\rho_m}{Q_w} \left(S D_b D_m N \right)^{1/2} (z_e - z_s) \right)$$

χ :	Devolatile efficiency
$z_e - z_s$:	Partial fill interval
ρ_m :	Melt density
Q_w :	Mass flux
D_b :	Barrel diameter
D_m :	Diffusion coefficient
N :	Rotation speed

Fig.9 Schematic illustration of Latinen's model*) for devolatilization in a single-screw extruder

*) Latinen, G.A. Devolatilization of viscous polymer systems. In Polymerization and Polycondensation Processes; American Chemical Society: Washington, DC, USA, 1962; Volume 34, pp. 235–246.

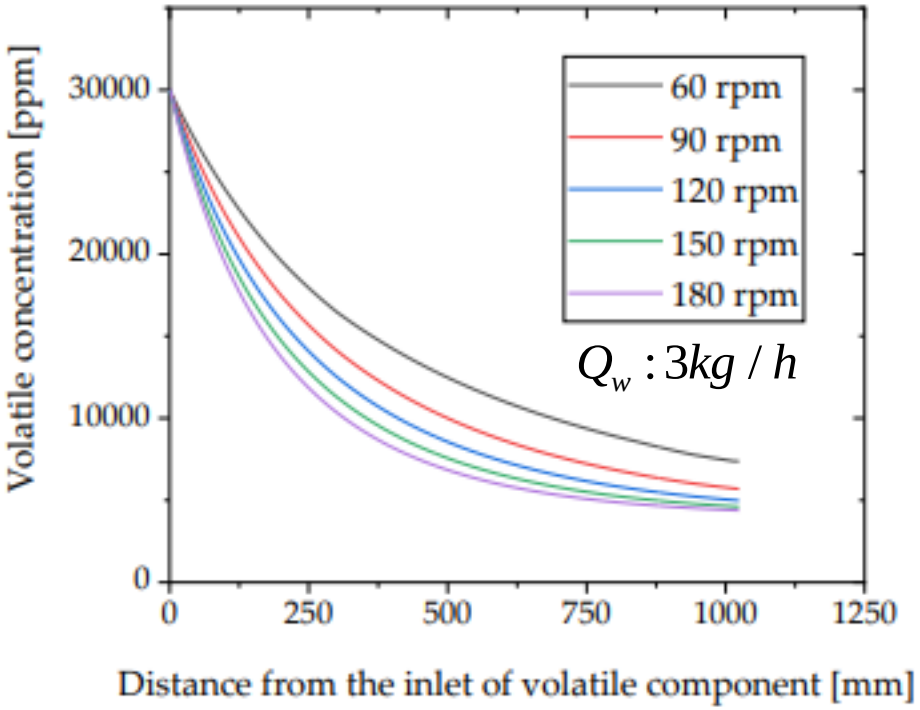
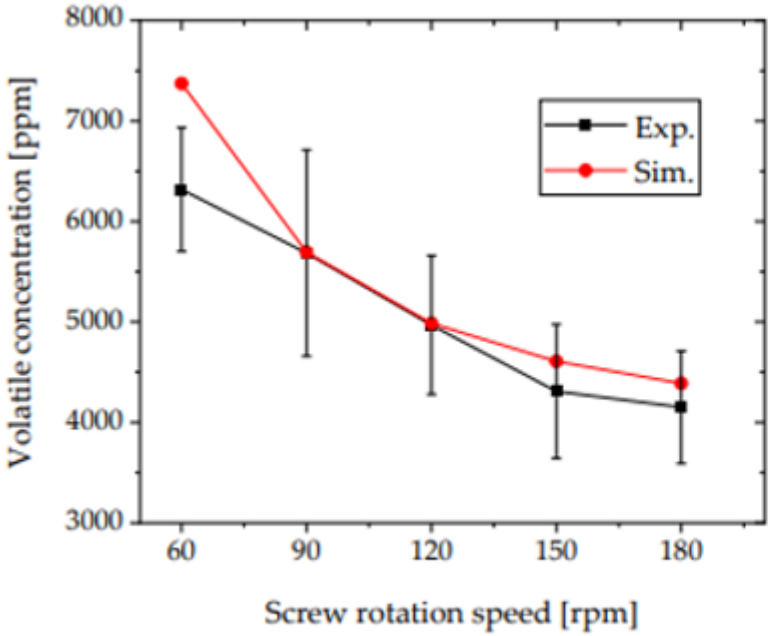
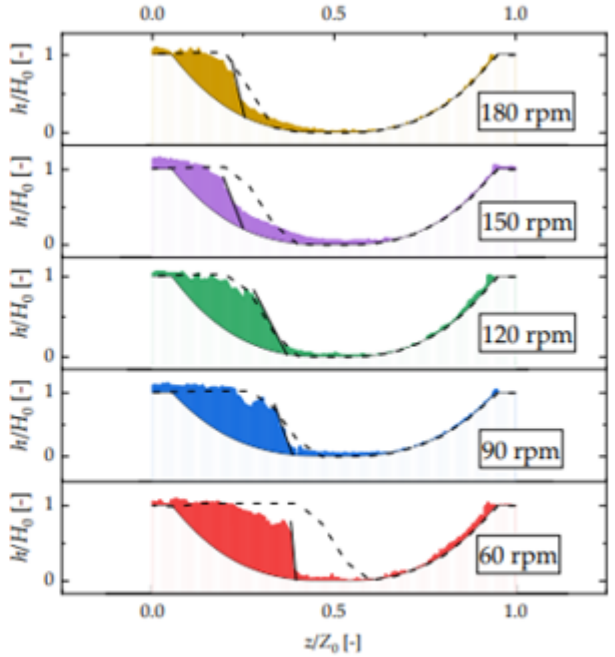


Fig.10 Simulation results of toluene concentration along the machine direction of twin screw extruder



(a) Volatile concentration

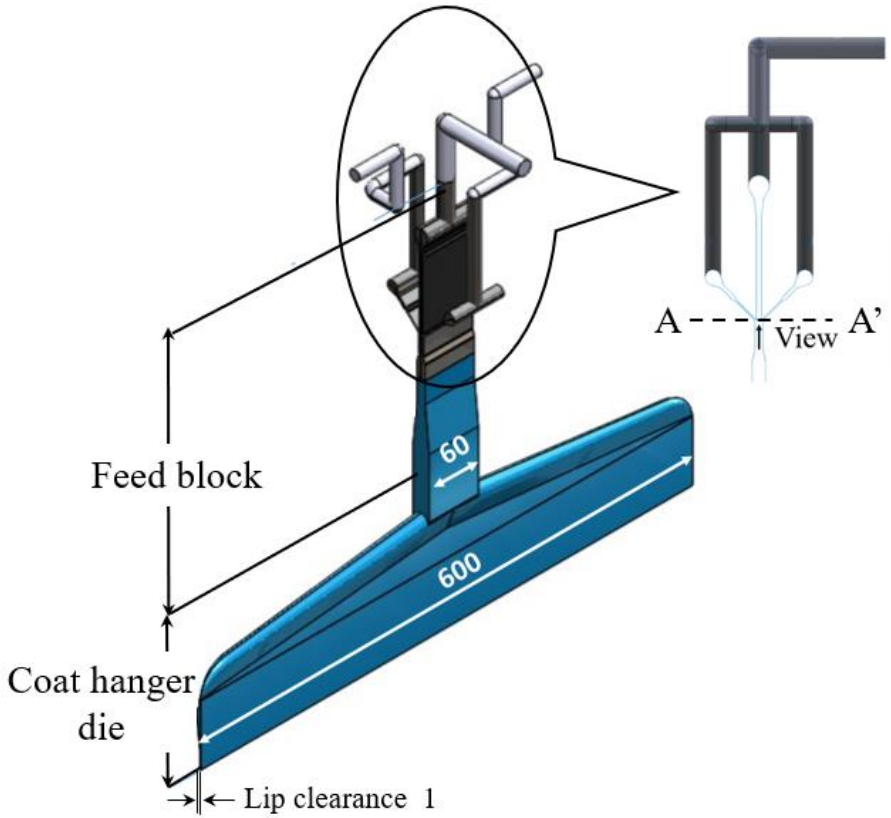


(b) Resin fill region

Fig.11 Comparison of the experiment and the predicted information ((a) volatile concentration, (b) resin fill region)

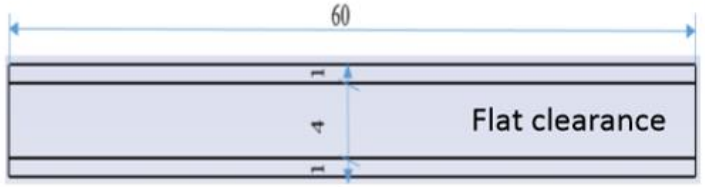
☐ Application for the multi extrusion die

「A Generalized 2.5D FEM Formulation for Steady Non-Newtonian Viscous Multi Flow : Part 1 & 2」[3),4)]

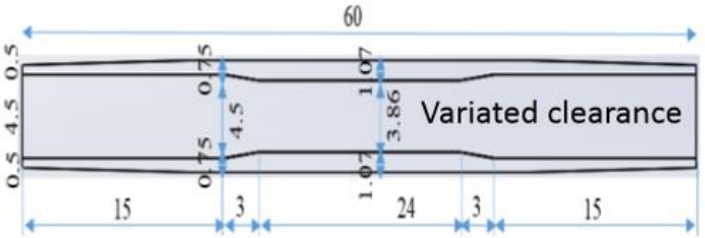


Surface layer : LDPE (LC720),4 kg/h,215℃

Mid layer : LDPE (LF405M),16 kg/h,215℃



(a) flat



(b) variated

Scale unit : [mm]

Fig. 12 Feed block type coat hanger die used in the experimental verification

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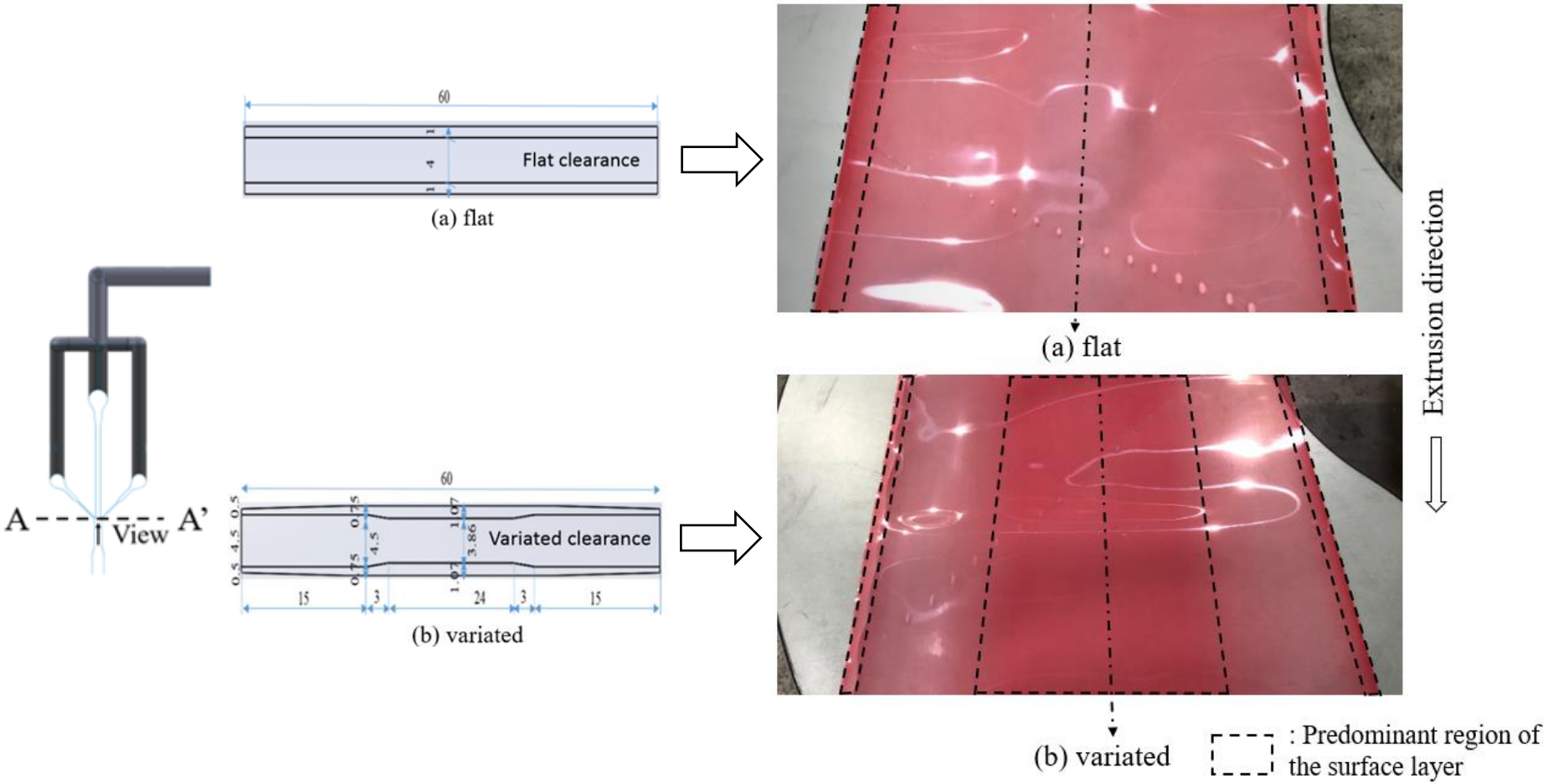
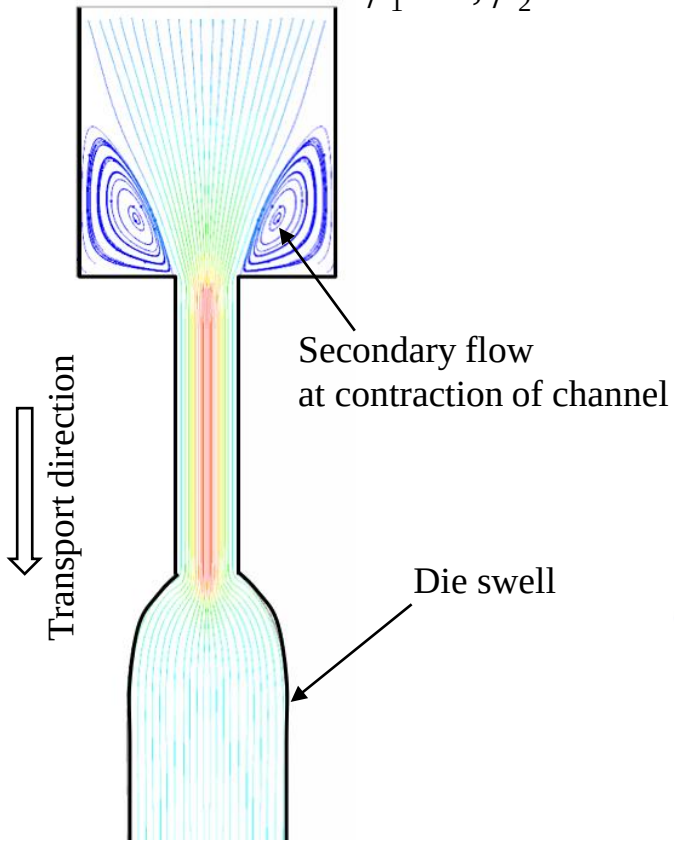


Fig. 13 Snapshots of the extruded multilayer film ((a) flat and (b) variated)

Viscoelastic phenomena neglected in the traditional 2.5D FEM

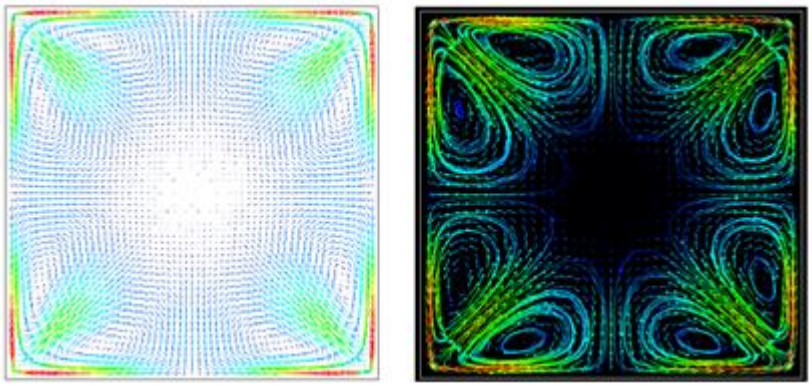
Main effecting factor :
first normal stress difference

$\psi_1 > 0, \psi_2 = 0$



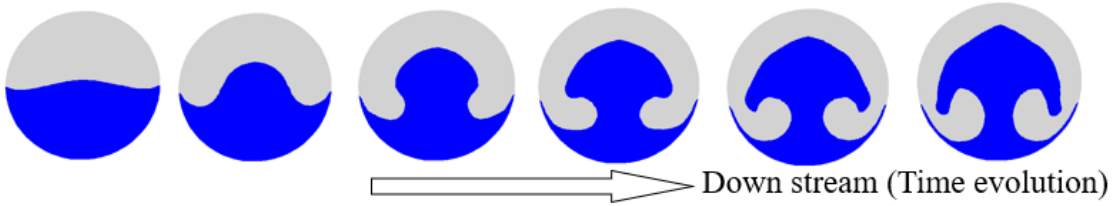
Main effecting factor :
second normal stress difference

$\psi_1 = 0, \psi_2 < 0$



Transport direction

Secondary flow in the rectangular cross section channel



Variation of multi layer flow interface in the circular cross section channel
(blue region : high viscosity flow, gray region : low viscosity flow)

Fig. 14 Various viscoelastic phenomena

Derivation of Pseudo Encapsulation Model

Governing equations

Momentum equation for creep flow

$$\nabla \bullet \boldsymbol{\sigma} = 0$$

CEF (Criminale Ericksen Filbey) model*)

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

Steady state

$u >> v, w$

Uniformity in machine direction $\dfrac{\partial \tau_{xx}}{\partial x} = \dfrac{\partial \tau_{xy}}{\partial x} = \dfrac{\partial \tau_{xz}}{\partial x} = 0$

Viscoelastic momentum equations

MD: Machine Direction

$$\frac{\partial p}{\partial x} = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} = \frac{\partial}{\partial y}\left(\eta \dot{\gamma}_{xy}\right) + \frac{\partial}{\partial z}\left(\eta \dot{\gamma}_{xz}\right)$$

Equivalent to viscous fluid equation

Thickness Direction

$$\frac{\partial p}{\partial y} = \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} = \frac{\partial}{\partial y}\left(\psi_2 \dot{\gamma}_{xy}^2\right) + \frac{\partial}{\partial z}\left(\psi_2 \dot{\gamma}_{xy} \dot{\gamma}_{xz}\right)$$

TD: Transverse Direction

$$\frac{\partial p}{\partial z} = \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} = \frac{\partial}{\partial y}\left(\psi_2 \dot{\gamma}_{xy} \dot{\gamma}_{xz}\right) + \frac{\partial}{\partial z}\left(\psi_2 \dot{\gamma}_{xz}^2\right)$$

Generates pressure gradient in each direction

$$\begin{cases} \dot{\gamma}_{xy} = \dfrac{\partial u}{\partial y} \\ \dot{\gamma}_{xz} = \dfrac{\partial u}{\partial z} \end{cases}$$

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

TD: Transverse Direction

$$\frac{\partial p}{\partial z}=\frac{\partial \tau_{xz}}{\partial x}+\frac{\partial \tau_{yz}}{\partial y}+\frac{\partial \tau_{zz}}{\partial z}=\frac{\partial}{\partial y}\left(\psi_2\dot{\gamma}_{xy}\dot{\gamma}_{xz}\right)+\frac{\partial}{\partial z}\left(\psi_2\dot{\gamma}_{xz}^2\right)$$

η, ψ_2, H : constant

Averaging in thickness direction

Using analytical solution of mono layer flow

Approximate representation of pressure

$$\langle p(z)\rangle=\langle p(0)\rangle+\psi_2\dot{\gamma}_W^2 g_f(z),$$

$$\dot{\gamma}_W=\left|\frac{W}{2\eta}\frac{\partial p}{\partial x}\right|,$$

$$g_f(z)=\frac{32}{\pi^4}\left(\frac{H}{W}\right)^2\sum_{n=1}^{\infty}\frac{1}{(2n-1)^4}\left(\frac{\sinh\left(\frac{(2n-1)\pi z}{H}\right)}{\cosh\left(\frac{(2n-1)\pi W}{2H}\right)}\right)^2$$

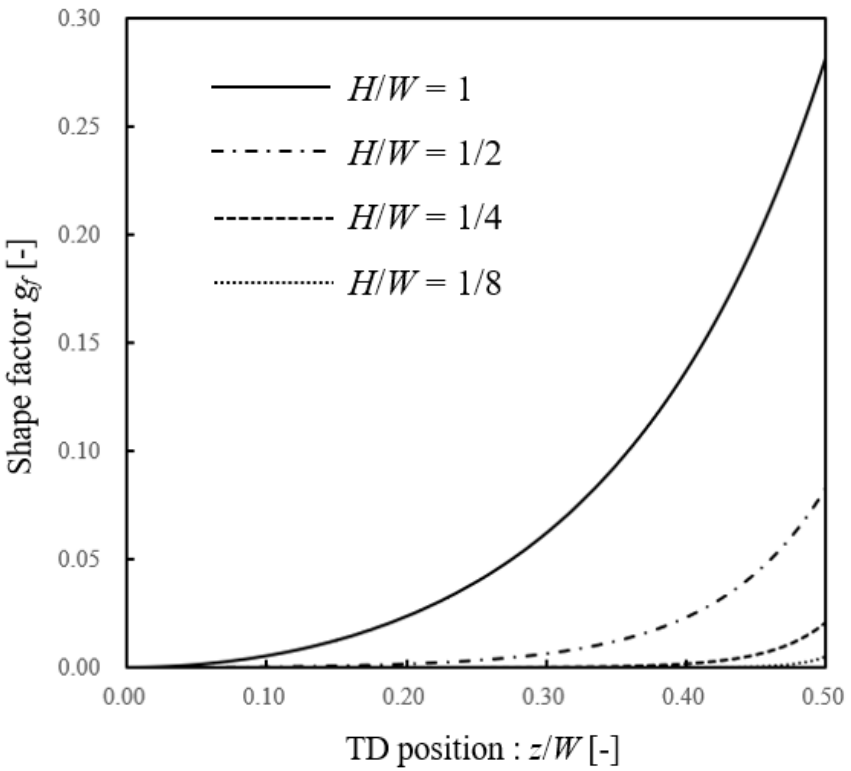
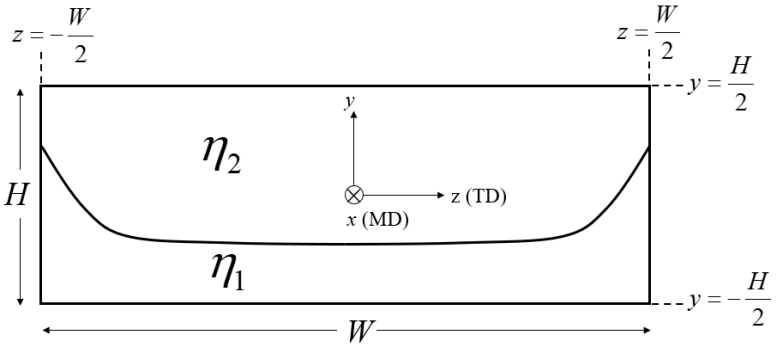


Fig. 15 Dependency of aspect ratio and TD position for the shape factor : g_f

Representation of the encapsulation using PEM



$$2\left(\frac{\eta_1}{h_1}+\frac{\eta_2}{h_2}\right)u\frac{\partial h_1}{\partial x}=\underbrace{p_1-p_2}+\underbrace{\left(\psi_{2,2}\left\langle\dot{\gamma}_{w2}^2\right\rangle-\psi_{2,1}\left\langle\dot{\gamma}_{w1}^2\right\rangle\right)g_f(z)}$$

$$\begin{cases} p_1 > p_2 \rightarrow \dfrac{\partial h_1}{\partial x} > 0 \\ p_1 < p_2 \rightarrow \dfrac{\partial h_1}{\partial x} < 0 \end{cases}$$

$$\begin{cases} \psi_{2,2}\left(\dfrac{1}{\eta_2}\dfrac{\partial p_2}{\partial x}\right)^2 > \psi_{2,1}\left(\dfrac{1}{\eta_1}\dfrac{\partial p_1}{\partial x}\right)^2 \rightarrow \dfrac{\partial h_1}{\partial x} > 0 \\ \psi_{2,2}\left(\dfrac{1}{\eta_2}\dfrac{\partial p_2}{\partial x}\right)^2 < \psi_{2,1}\left(\dfrac{1}{\eta_1}\dfrac{\partial p_1}{\partial x}\right)^2 \rightarrow \dfrac{\partial h_1}{\partial x} < 0 \end{cases}$$

Assumption: $p_1 \cong p_2$,

$$\lambda=\frac{\eta_1}{\eta_2}\cong\frac{\psi_{2,1}}{\psi_{2,2}}<1 \quad ?$$

$$\Rightarrow \quad \lambda^2<\lambda \rightarrow \frac{\partial h_1}{\partial x}>0$$

Low-viscosity fluid encapsulates high-viscosity fluid under limited condition.

!!!

2.5D FEM model

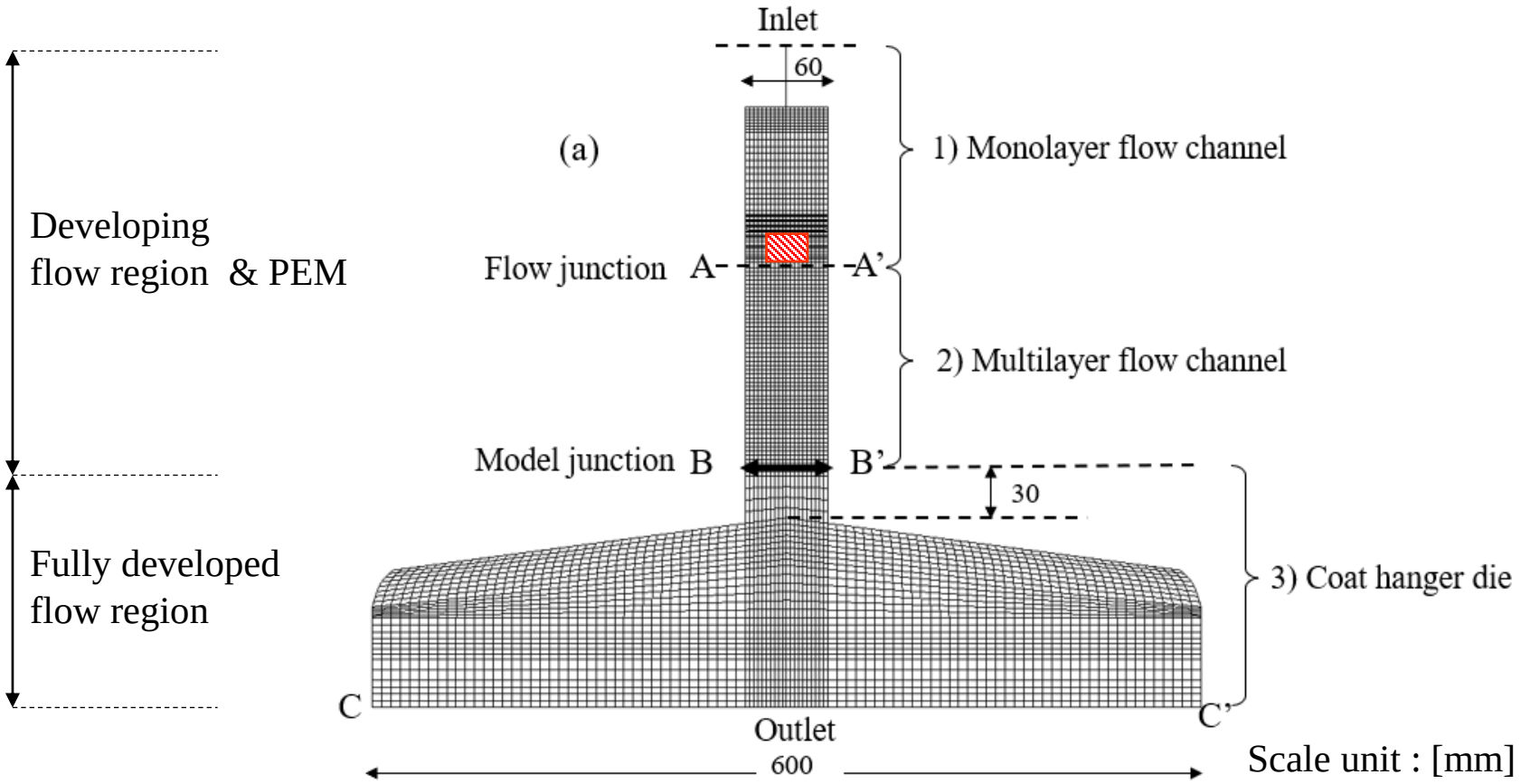
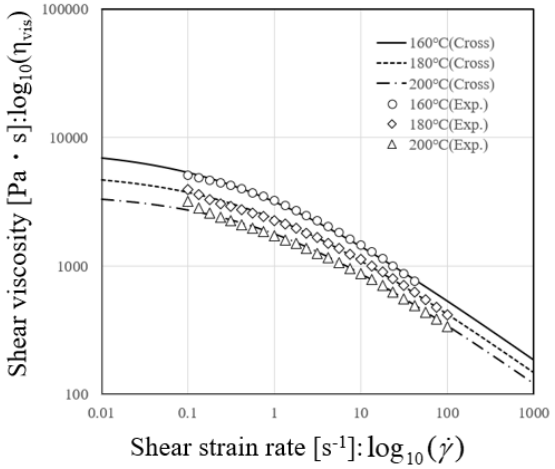


Fig. 16 Multi layer flow analysis model

Material properties

(a) LC720
Surface layer



(b) LF405M
Mid layer

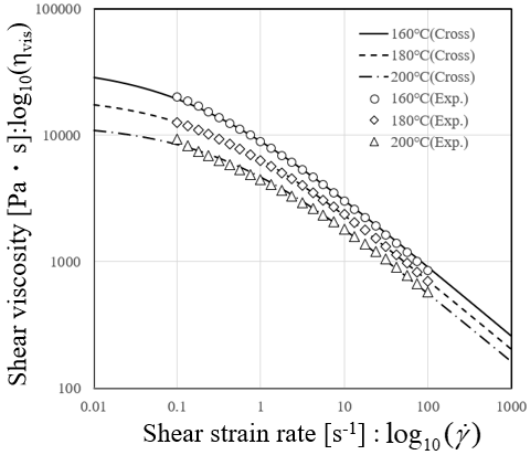
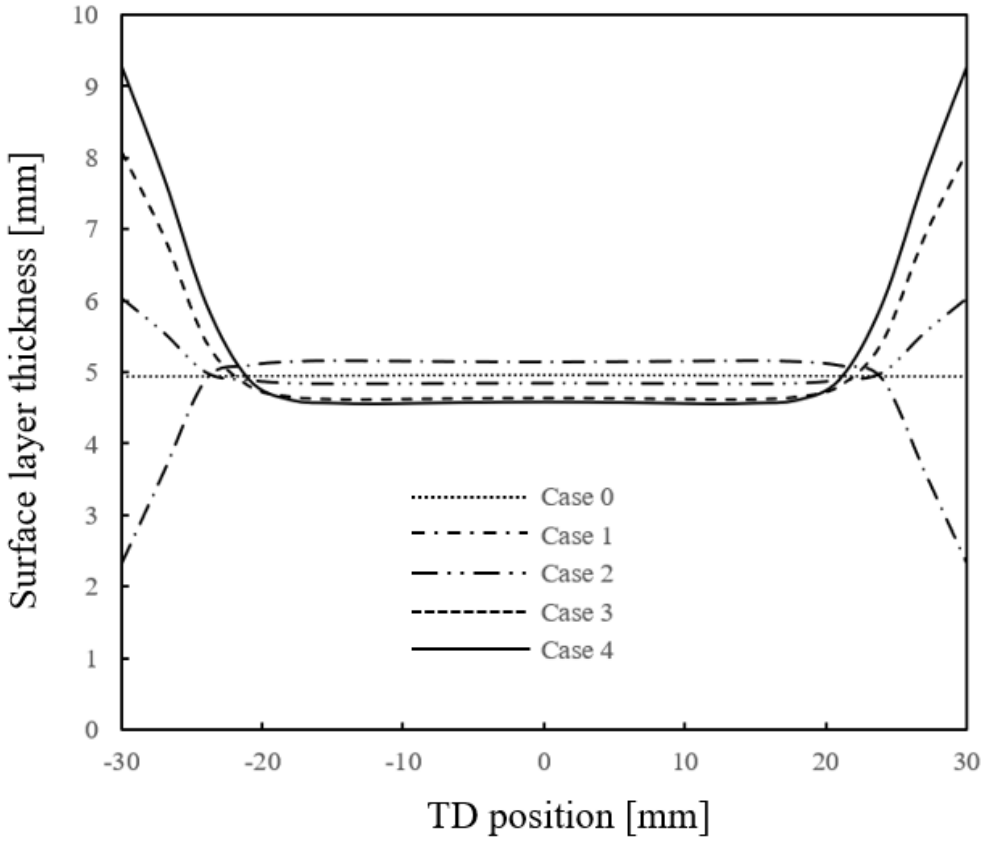


Table 1 Second normal difference coefficients of PEM

Case	Second normal stress difference coefficient : Ψ_2 [Pa・s^2] Layer 1	Layer 2	Layer 3
0	0	0	0
1	0	-60	0
2	-8	-60	-8
3	-10	-60	-10
4	-18	-60	-18

LDPE (LC720,LF405M)
supplied by Japan Polyethylene Corp.

Fig.17 Flow curve fitted using the Cross model



$\psi_2 \left[Pa \bullet s^2 \right]$

	Layer1	Layer 2	Layer3
Case4 :	-18	-60	-18
Case1 :	0	-60	0
Case0 :	0	0	0

Fig. 18 Predicted surface layer thickness at the outlet position (B-B') of the feed block channel under the flat condition

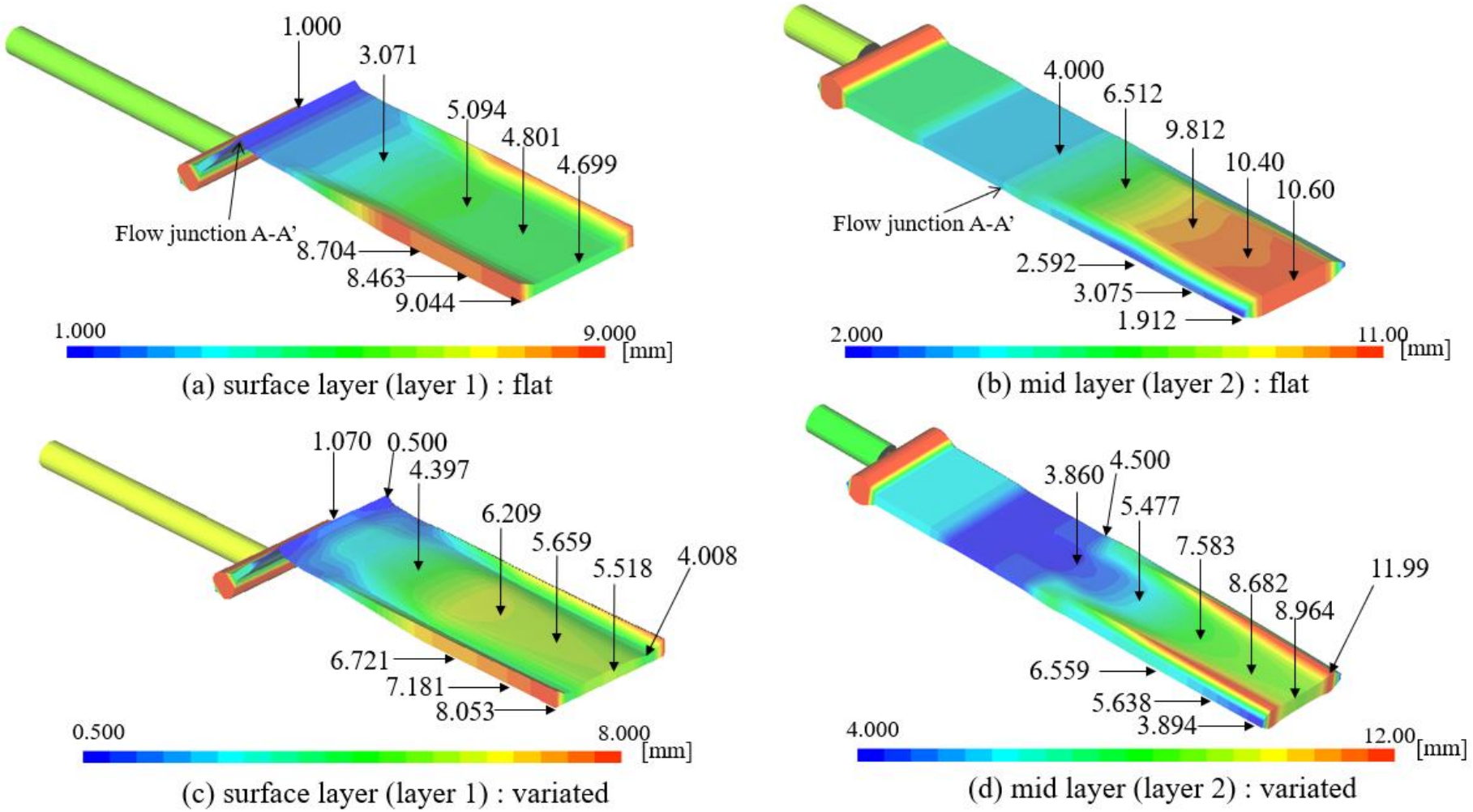
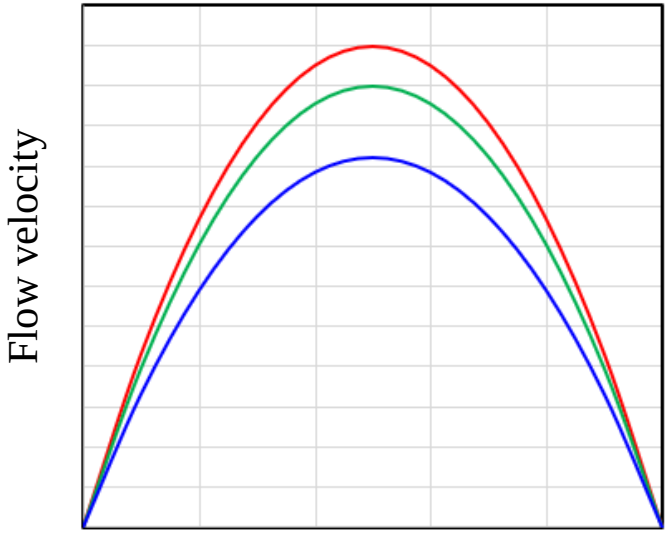


Fig. 19 Predicted layer thickness ((a) surface layer, (b) mid layer : flat and (c) surface layer, (d) mid layer : variated)

Mysterious nature of multi layer flow

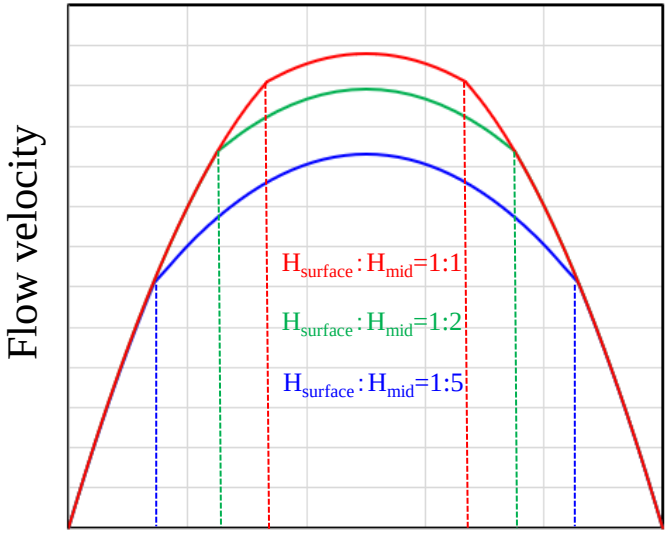
Mono layer flow



$\Delta p < \Delta p < \Delta p$

$$\because \Delta p = \frac{2\eta\dot{\gamma}_w}{H}$$

Multi layer flow ($\eta_{surafce} < \eta_{mid}$)



$\Delta p = \Delta p = \Delta p$!!!

$$\chi_h^4 = -4\chi_\eta\chi_h^3 - 3(\chi_\eta - \chi_q\chi_\eta)\chi_h^2 + 4\chi_q\chi_\eta\chi_h + \chi_q\chi_\eta^2$$

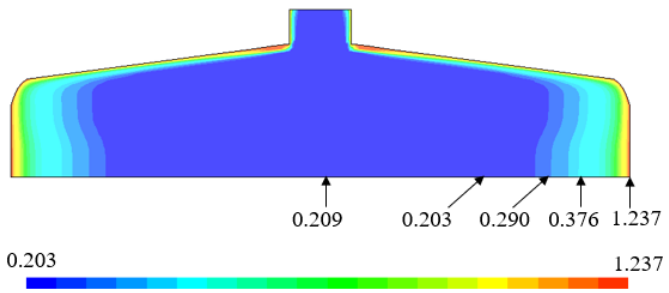
for two layer flow under fully developed state

$$\frac{\partial}{\partial x_i}\left(S_l \frac{\partial p_l}{\partial x_i}\right) = F_l \quad \Rightarrow \quad v_{mi}\frac{\partial \chi_{qlm}}{\partial x_i} = 0$$

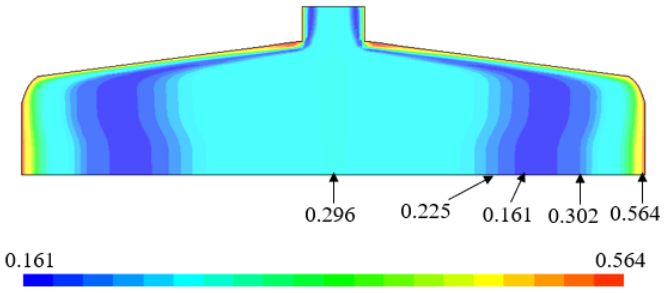
Elliptic type Diffusion

$p_l = p$ *for* $l = 1 \sim n$

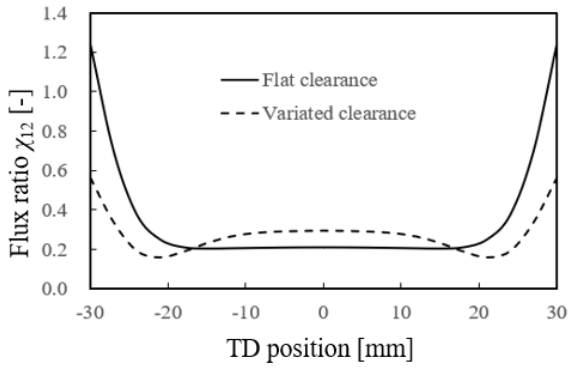
hyperbolic type Convection



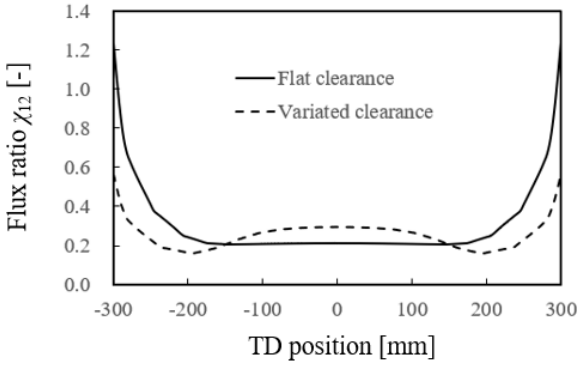
(a) flat



(b) variated



(c) inlet



(d) outlet

Fig. 20 Predicted flux ratio $\chi_{12}(= q_1/q_2 = \chi_{32})$: contour plot of (a) flat and (b) variated , graph plot of (c) inlet (B-B') and (d) outlet (C-C')

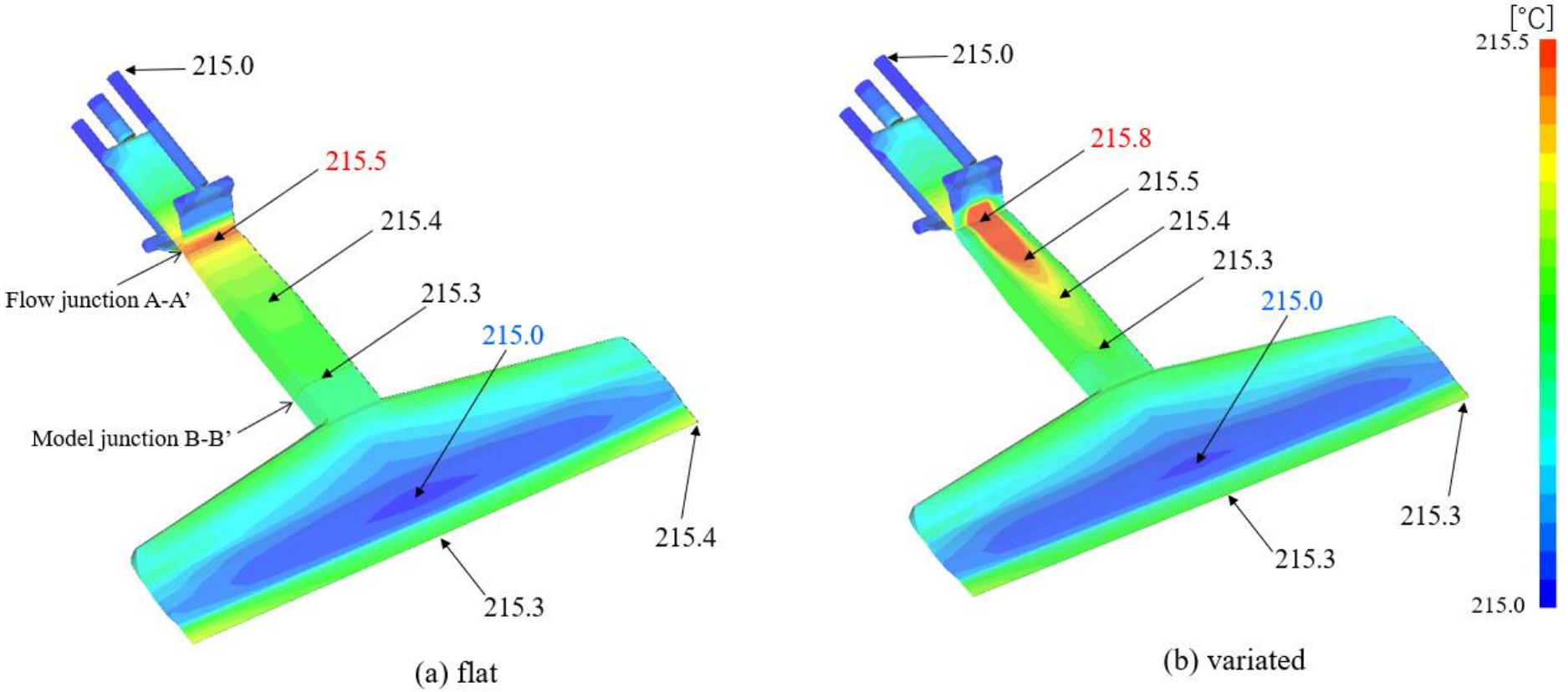
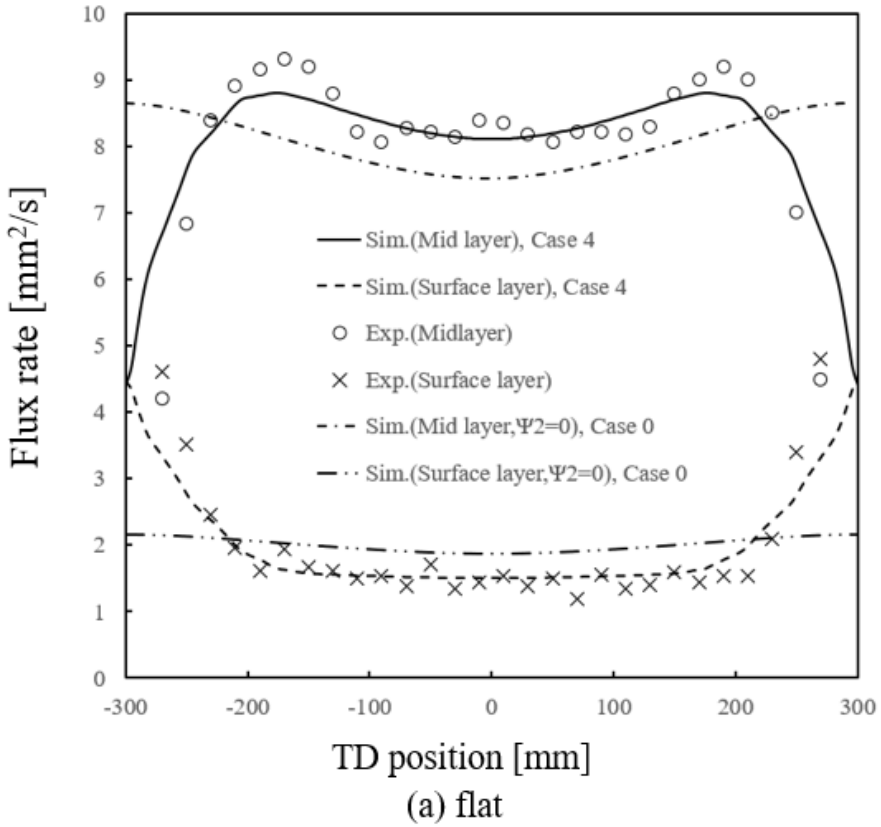


Fig. 21 Comparison of the predicted pressure ((a) flat and (b) variated)



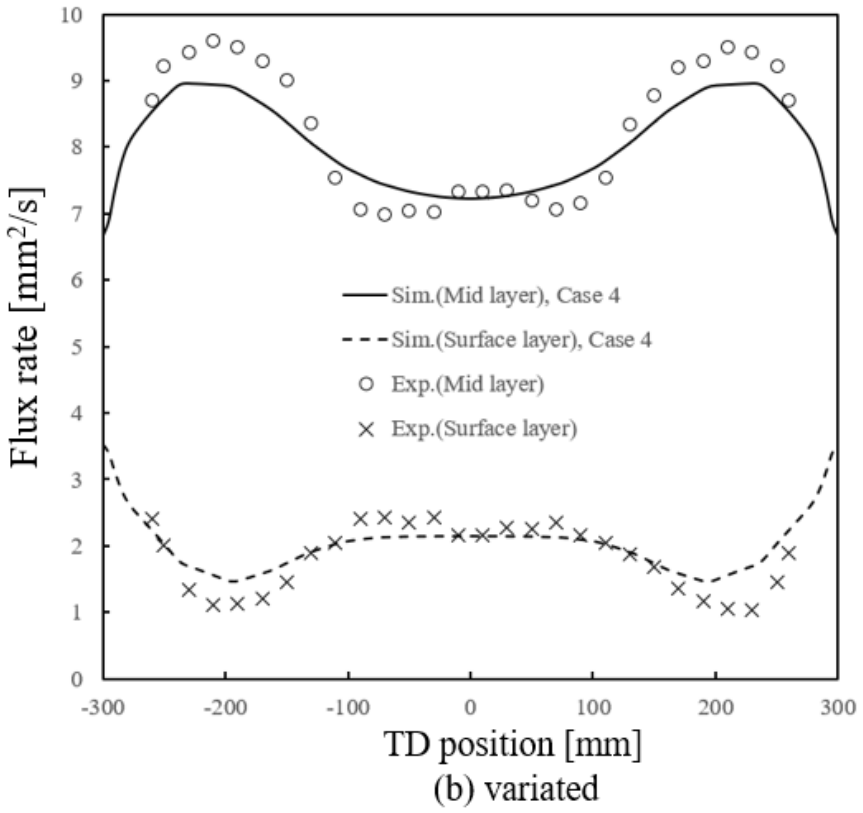


Fig. 22 Comparison of the measured and the predicted flux rate at the die outlet position (C-C'), ((a) flat and (b) variated)

☐Conclusions

・Various phenomena in the polymer extrusion process can be quantified in a short compulational time with an easy operation using 2.5D FEM.

・The unfilled state in the twin screw extruder can be represented with moderate accuracy by the pressure rearrangement algorithm.

・The implementation of PEM reduces the discrepancy between the predicted layer thickness and the measured value in a feed block type coat hanger die.

❑Future prospections

「Experimental Investigation and Numerical Simulation of a Self-Wiping Corotating Parallel Octa-Screw Extruder」[5)]

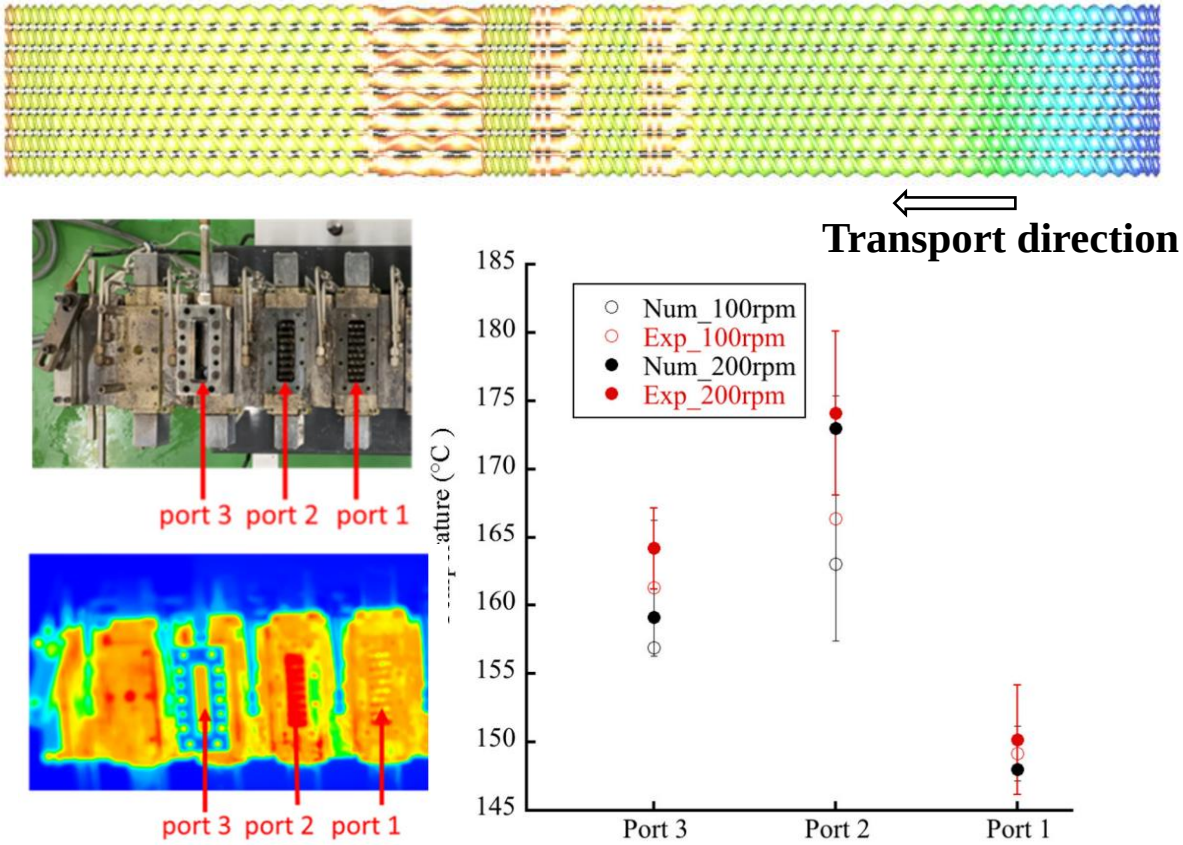


Fig. 23 Measured and calculated temperature distribution in an octa screw extruder

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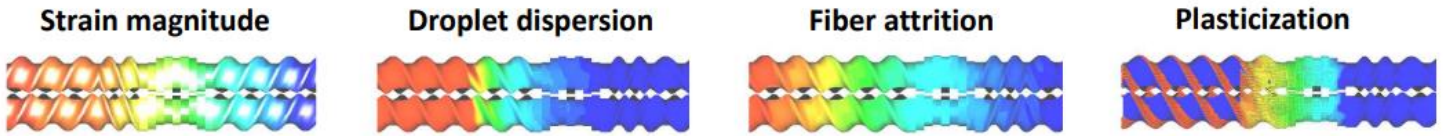
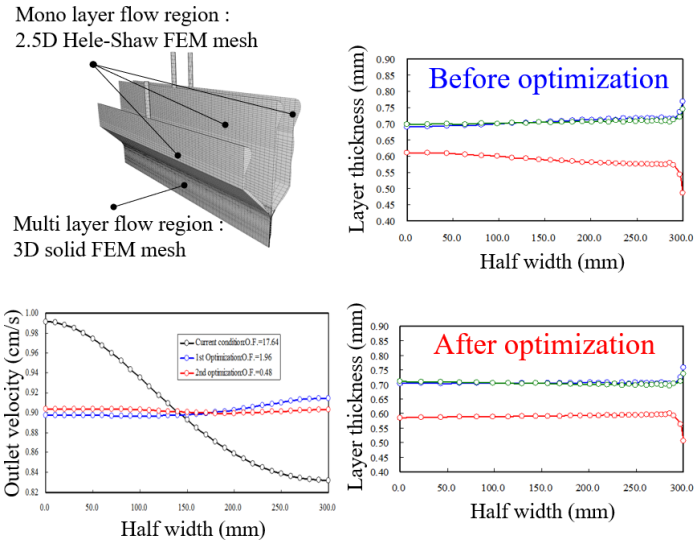
Experimental verifications and enhancement of applications

For screw extruder

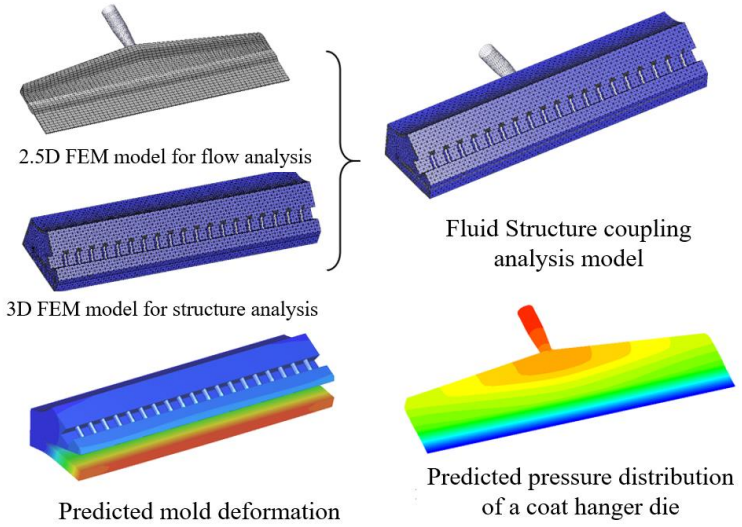


Side feed, Reactive extrusion, etc.

For multilayer extrusion die



Optimization analysis of a multi manifold die



Fluid/Structure coupling analysis

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