8:00-8:30am 30 min.

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Fill ratio distribution in a co-rotating self-wiping twin screw extruder—theoretical and experimental study

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Agenda

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1. Introduction
2. Theory and formulation
3. Algorithm for fill ratio distribution
4. Conclusion

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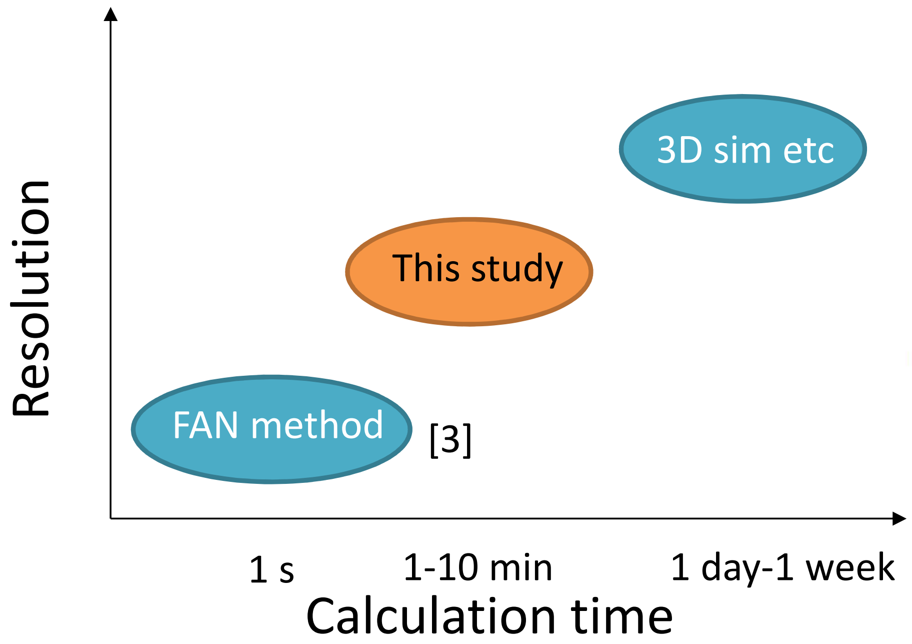
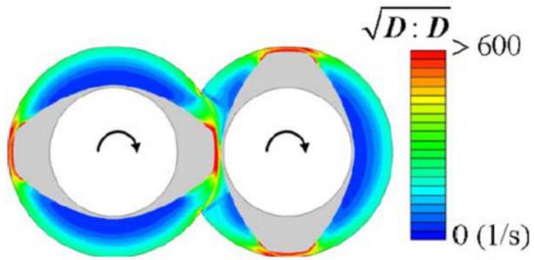
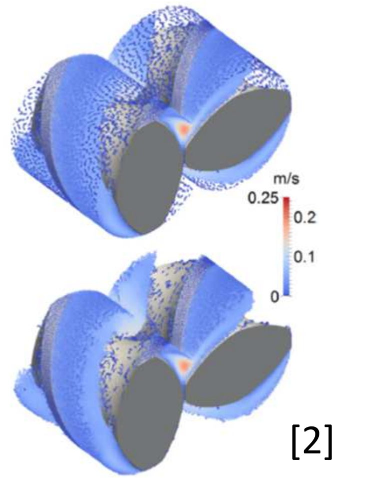
Numerical Simulation of TSE





[1]

Figure 2. Distribution of $\sqrt{D:D}$ as a typical magnitude of the strain rate at position B in Figure 1.



[2]

Fig. 12. Snapshots of the half-filled screw element and axial velocity distribution (clockwise rotation). Top: including all particles, bottom: suppressing particles at the barrel wall.

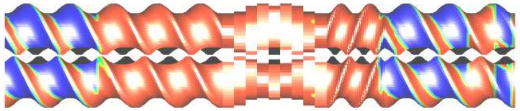
1. Yasuya Nakayama, Toshihisa Kajiwara, Tatsunori Masaki, AIChE J, 62(7), 2563-2569 (2016).b
2. Andreas Eitzlmayr, Johannes Khinast, Chemical Engineering Science, 134, 861-879 (2015).
3. Tadmor, Z., Broyer, E. and Gutfinger, C.: Polym. Eng. Sci., 14,660(1984)
4. Broyer, E., Gutfinger, C. and Tadmor Z. : Trans. Soc. Rheology, 19, 423(1975)
5. J. L. White, Z. Y. Chen, Polymer Engineering and Science, 34(3), 229-237 (1994).
6. Santosh Bawiskar, James L. White, Polymer Engineering & Science, 38(5), 727-740 (1998).
7. James L. White, Eung Kyu Kim, Jong Min Keum, Ho Chul Jung, Dae Suk Bang, Polymer Engineering & Science, 41(8), 1448-1455 (2001).
8. J. L. White, B. J. Kim, S. Bawiskar, J. M. Keum, Polymer-Plastics Technology and Engineering, 40(4), 385-405 (2001).

What our simulator can do.

Hele-Shaw flow model + finite element method

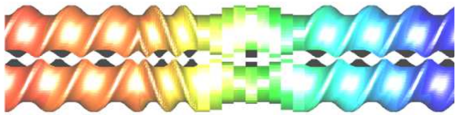
Pressure distribution

Fill ratio distribution

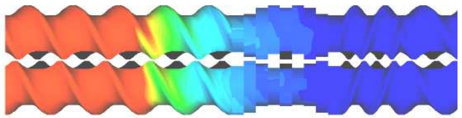


Strain rate, velocity, flow rate distribution on whole screw elements

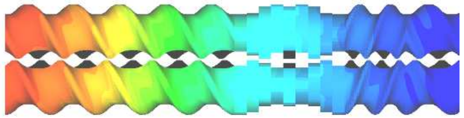
Strain magnitude



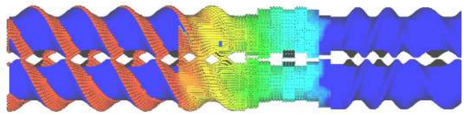
Droplet dispersion



Fiber attrition



Plasticization



Advantage of our software

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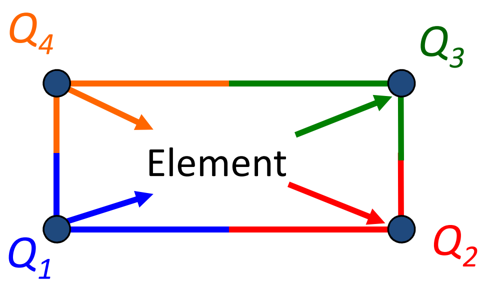
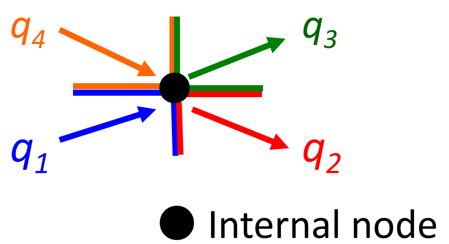
1. **Calculation cost is low** as the pressure is the only unknown variable to be determined for isothermal condition.
2. **It is easy to calculate flow metrics;** velocity, strain rate, viscosity distribution by the integration along the thickness (r direction) when the pressure and temperature are determined.
3. **Flow balance satisfies with high-precision.**



The total flow rate at a node becomes zero for any values of pressure.

$$\sum_{\alpha=1}^{4} Q_\alpha = 0 \qquad \because \sum_{\alpha=1}^{4} \phi_\alpha = 1$$



The summation of flow rate for internal nodes calculated by the pressure becomes zero.

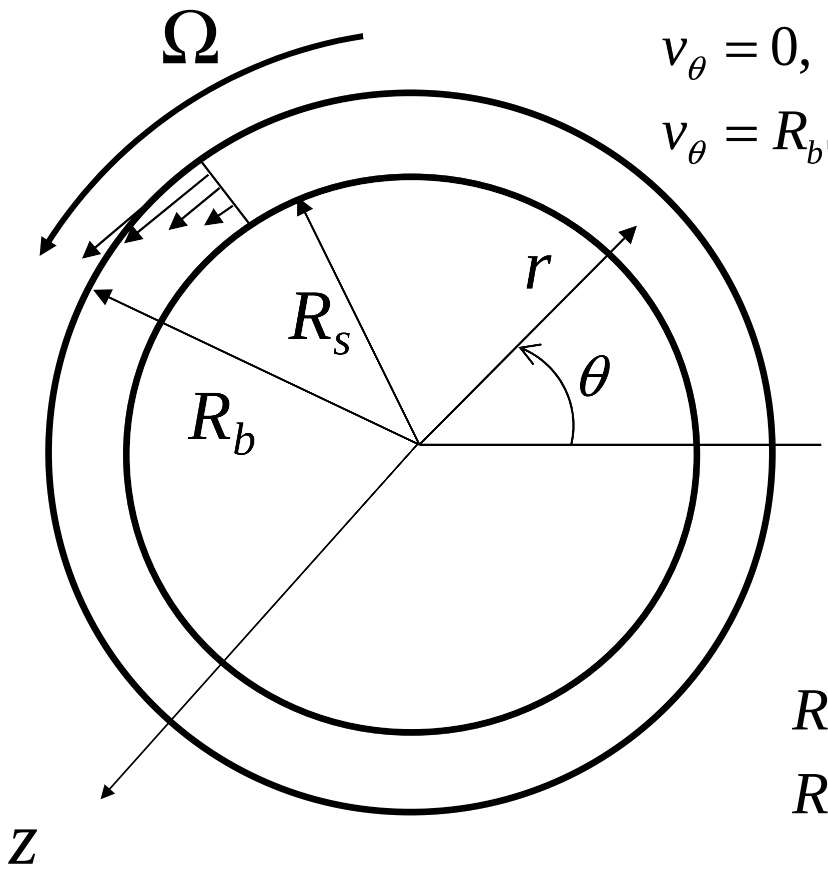
$$\sum_{\alpha=1}^{4} q_\alpha = 0$$

Hele-Shaw flow 2.5D model in cylinder

$v_r = 0$, v_z and v_θ are solo function of r.

$$v_\theta = 0,\ v_z = 0\ at\ r = R_s$$

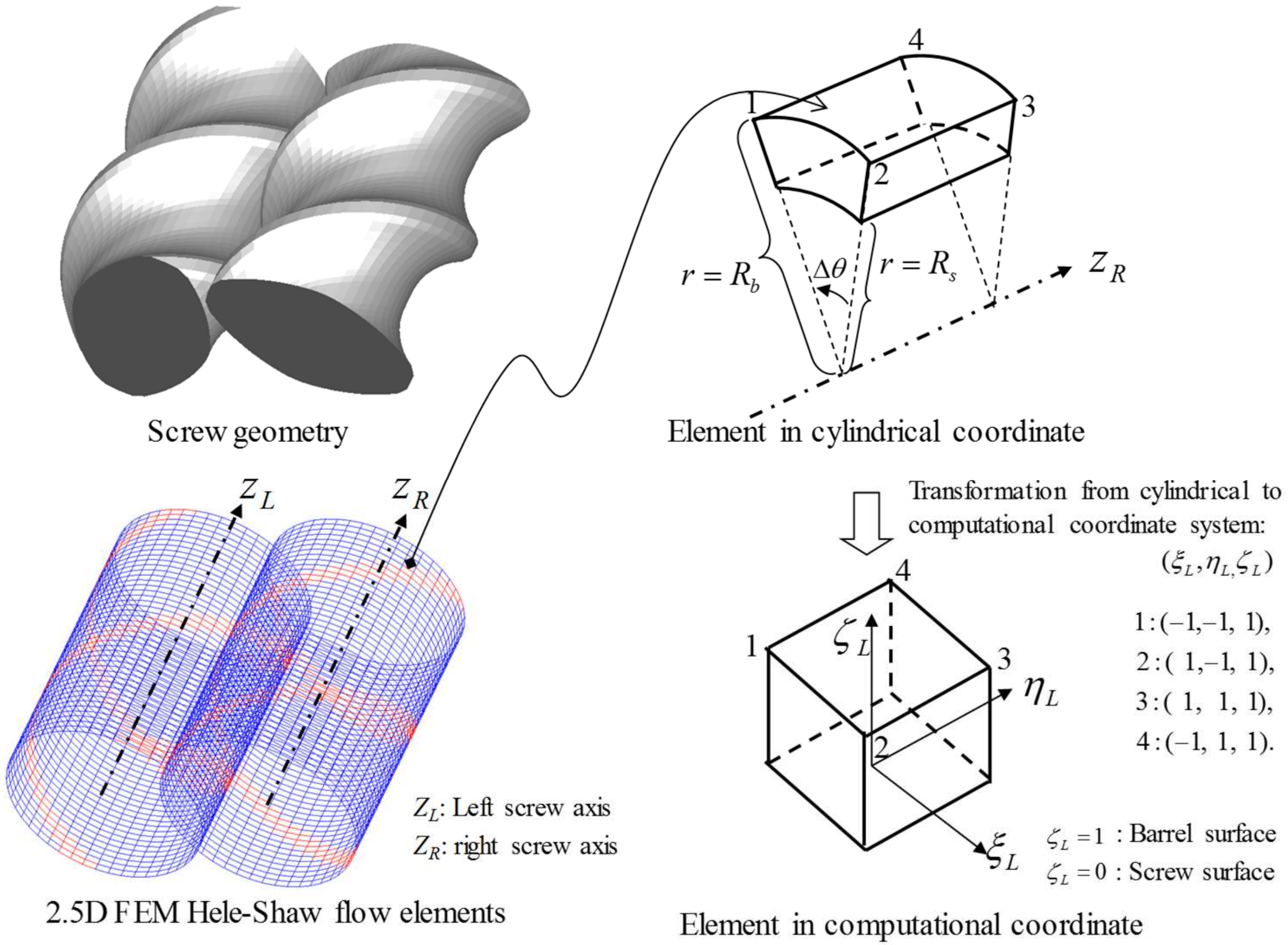
$$v_\theta = R_b\Omega,\ v_z = 0\ at\ r = R_b$$



R_s: Screw radius

R_b: Barrel radius

Geometry

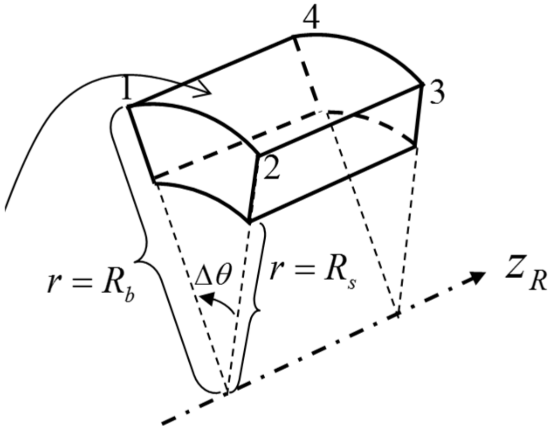


Screw geometry
Element in cylindrical coordinate
1
2
3
4
$r = R_b$
$\Delta\theta$
$r = R_s$
z_R
z_L
z_R
Transformation from cylindrical to computational coordinate system:
(ξ_L, η_L, ζ_L)
$1: (-1, -1, 1)$,
$2: (1, -1, 1)$,
$3: (1, 1, 1)$,
$4: (-1, 1, 1)$.
ζ_L
η_L
ξ_L
$\zeta_L = 1$: Barrel surface
$\zeta_L = 0$: Screw surface
Z_L: Left screw axis
Z_R: right screw axis
2.5D FEM Hele-Shaw flow elements
Element in computational coordinate

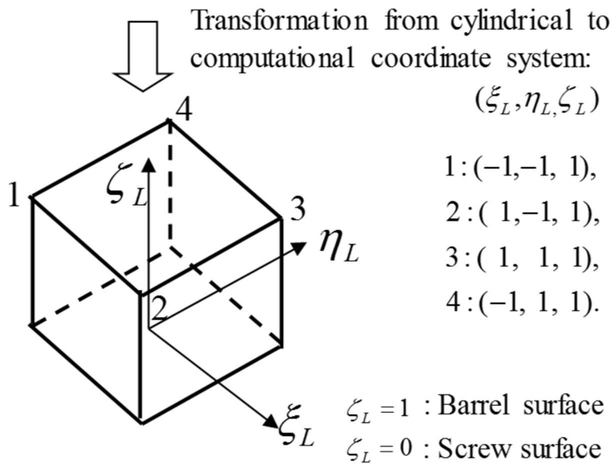
Shape function

$$p=\sum_{\alpha=1}^{4}\phi_\alpha p_\alpha,\ \ \theta=\sum_{\alpha=1}^{4}\phi_\alpha\theta_\alpha,\ \ z=\sum_{\alpha=1}^{4}\phi_\alpha z_\alpha,\ \ r=\left(R_b-R_s\right)\zeta_L+R_s$$

$$\phi_1=\frac{1}{4}\left(1-\xi_L\right)\left(1-\eta_L\right),\ \phi_2=\frac{1}{4}\left(1+\xi_L\right)\left(1-\eta_L\right),\phi_3=\frac{1}{4}\left(1+\xi_L\right)\left(1+\eta_L\right),\ \phi_4=\frac{1}{4}\left(1-\xi_L\right)\left(1+\eta_L\right)$$



Element in cylindrical coordinate



Element in computational coordinate

Eq. of Continuity in cylindrical coordinate

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As ρ = constant and $v_r = 0$,

$$\cancel{\frac{\partial \rho}{\partial t}} + \cancel{\frac{1}{r}\frac{\partial}{\partial r}(\rho r v_r)} + \frac{1}{r}\frac{\partial}{\partial \theta}(\rho v_\theta) + \frac{\partial}{\partial z}(\rho v_z) = 0$$

$$\Downarrow$$

$$\frac{1}{r}\frac{\partial}{\partial \theta}(\rho v_\theta) + \frac{\partial}{\partial z}(\rho v_z) = 0$$

Eq. of Motion

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θ-component

As steady state, $\partial v_\theta/\partial\theta = \partial v_\theta/\partial z = 0$, $v_r = 0$,

$$\frac{\partial}{\partial r}\left(\frac{\eta}{r}\frac{\partial}{\partial r}(r v_\theta)\right) + \frac{\eta}{r^2}\cancel{\frac{\partial^2 v_\theta}{\partial \theta^2}} + \eta\cancel{\frac{\partial^2 v_\theta}{\partial z^2}} + \frac{2\eta}{r^2}\cancel{\frac{\partial v_r}{\partial \theta}} = \frac{1}{r}\frac{\partial p}{\partial \theta}$$

$$\Downarrow$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\eta\left(\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r}\right)\right) = \frac{1}{r}\boxed{\frac{\partial p}{\partial \theta}}$$

Eq. of Motion (Cont')

z-component

As steady state, $\partial v_z/\partial\theta = \partial v_z/\partial z = 0$,

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\eta\frac{\partial v_z}{\partial r}\right)+\frac{\eta}{r^2}\cancel{\frac{\partial^2 v_z}{\partial\theta^2}}+\eta\cancel{\frac{\partial v_z}{\partial z^2}}=\frac{\partial p}{\partial z}$$

$$\Downarrow$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\eta\frac{\partial v_z}{\partial r}\right)=\boxed{\frac{\partial p}{\partial z}}$$

Strain rate

***θr*-component**

$$\dot{\gamma}_{\theta r} \equiv r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right) = \frac{1}{2\eta}\left(\boxed{\frac{\partial p}{\partial \theta}}\right)\left(1-\frac{1}{r^2}\left(\frac{\Omega}{\gamma_c}\right)\right)+\frac{1}{\eta r^2}\left(\frac{\Omega}{\gamma_c}\right)$$

***zr*-component**

$$\dot{\gamma}_{zr} \equiv \frac{\partial v_z}{\partial z} = \frac{1}{2\eta}\left(\boxed{\frac{\partial p}{\partial z}}\right)\left(r-\frac{1}{r}\left(\frac{\alpha_c}{\beta_c}\right)\right)$$

Integration constant

$$\alpha_c = \int_{R_s}^{R_b}\frac{r}{\eta}dr,\ \ \beta_c = \int_{R_s}^{R_b}\frac{1}{\eta r}dr,\ \ \gamma_c = \int_{R_s}^{R_b}\frac{1}{\eta r^3}dr,\ \ \delta_c = \int_{R_s}^{R_b}\frac{r^3}{\eta}dr$$

Velocity

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θ-component

$$v_\theta = \frac{r}{2}\left(\boxed{\frac{\partial p}{\partial \theta}}\right)\left(\int_{R_s}^{r}\frac{1}{\eta r}dr - \left(\frac{\beta_c}{\gamma_c}\right)\int_{R_s}^{r}\frac{1}{\eta r^3}dr\right) + \left(\frac{\Omega r}{\gamma_c}\right)\int_{R_s}^{r}\frac{1}{\eta r^3}dr$$

z-component

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

Integration constant

$$\alpha_c = \int_{R_s}^{R_b}\frac{r}{\eta}dr,\ \ \beta_c = \int_{R_s}^{R_b}\frac{1}{\eta r}dr,\ \ \gamma_c = \int_{R_s}^{R_b}\frac{1}{\eta r^3}dr,\ \ \delta_c = \int_{R_s}^{R_b}\frac{r^3}{\eta}dr$$

Flow rate

θ-component $$q_\theta \equiv \int_{R_s}^{R_b} v_\theta dr = -\frac{1}{4}\left(\boxed{\frac{\partial p}{\partial \theta}}\right)\left(\alpha_c - \frac{\beta_c^2}{\gamma_c}\right) + \frac{\Omega}{2}\left(R_b^2 - \frac{\beta_c}{\gamma_c}\right)$$

z-component $$q_z \equiv \int_{R_s}^{R_b} v_z r dr = -\frac{1}{4}\boxed{\frac{\partial p}{\partial z}}\left(\delta_c - \frac{\alpha_c^2}{\beta_c}\right)$$

Integration constant

$$\alpha_c = \int_{R_s}^{R_b} \frac{r}{\eta} dr, \quad \beta_c = \int_{R_s}^{R_b} \frac{1}{\eta r} dr, \quad \gamma_c = \int_{R_s}^{R_b} \frac{1}{\eta r^3} dr, \quad \delta_c = \int_{R_s}^{R_b} \frac{r^3}{\eta} dr$$

Flow balance of each element

$$Q_\alpha^e = -\left(S_{\alpha\beta}^{e\theta} + S_{\alpha\beta}^{ez}\right)\boxed{p_\beta^e} + D_\alpha^e$$

Flow through a node of element

Pressure-gradient driven flow

Drag-force driven flow

$$Q_\alpha^e = \int_{\Gamma_e} \phi_\alpha (n_\theta q_\theta + n_z q_z) d\Gamma, \quad S^\theta = \frac{1}{4}\left(\alpha_c - \frac{\beta_c^2}{\gamma_c}\right), \quad S^z = \frac{1}{4}\left(\delta_c - \frac{\alpha_c^2}{\beta_c}\right),$$

$$S_{\alpha\beta}^{e\theta} = S^\theta \int_{S_e} \frac{\partial \phi_\alpha}{\partial \theta}\frac{\partial \phi_\beta}{\partial \theta} dS, \quad S_{\alpha\beta}^{ez} = S^z \int_{S_e} \frac{\partial \phi_\alpha}{\partial z}\frac{\partial \phi_\beta}{\partial z} dS, \quad D^\theta = \frac{\Omega}{2}\left(R_b^2 - \frac{\beta_c}{\gamma_c}\right)$$

$$D_\alpha^e = D^\theta \int_{S_e} \frac{\partial \phi_\alpha}{\partial \theta} dS$$

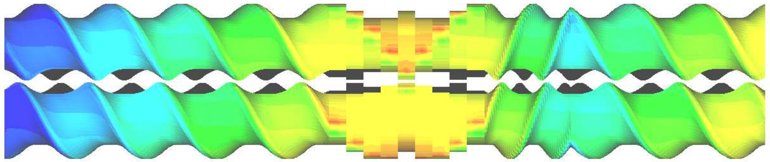
$$\alpha_c = \int_{R_s}^{R_b} \frac{r}{\eta} dr, \quad \beta_c = \int_{R_s}^{R_b} \frac{1}{\eta r} dr, \quad \gamma_c = \int_{R_s}^{R_b} \frac{1}{\eta r^3} dr, \quad \delta_c = \int_{R_s}^{R_b} \frac{r^3}{\eta} dr$$

$$\phi_1 = \frac{1}{4}(1-\xi_L)(1-\eta_L), \quad \phi_2 = \frac{1}{4}(1+\xi_L)(1-\eta_L), \phi_3 = \frac{1}{4}(1+\xi_L)(1+\eta_L), \quad \phi_4 = \frac{1}{4}(1-\xi_L)(1+\eta_L)$$

Filled and unfilled calculation

Completely filled screws

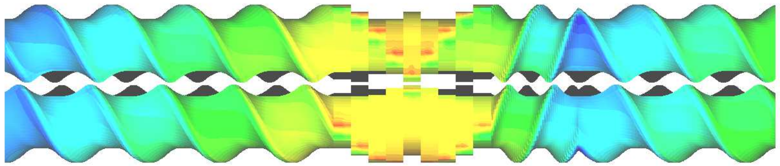
Press. at feed
0MPa（given）



Head press.
10MPa（given）

Q = 20kg/h (Calc. result)

Press. at feed
0MPa（given）



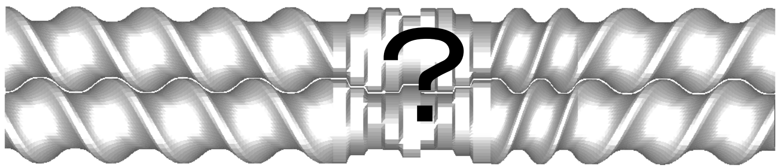
Head press.
5MPa（given）

Q = 40kg/h (Calc. result)

One degree of freedom is added.

Partially filled screw

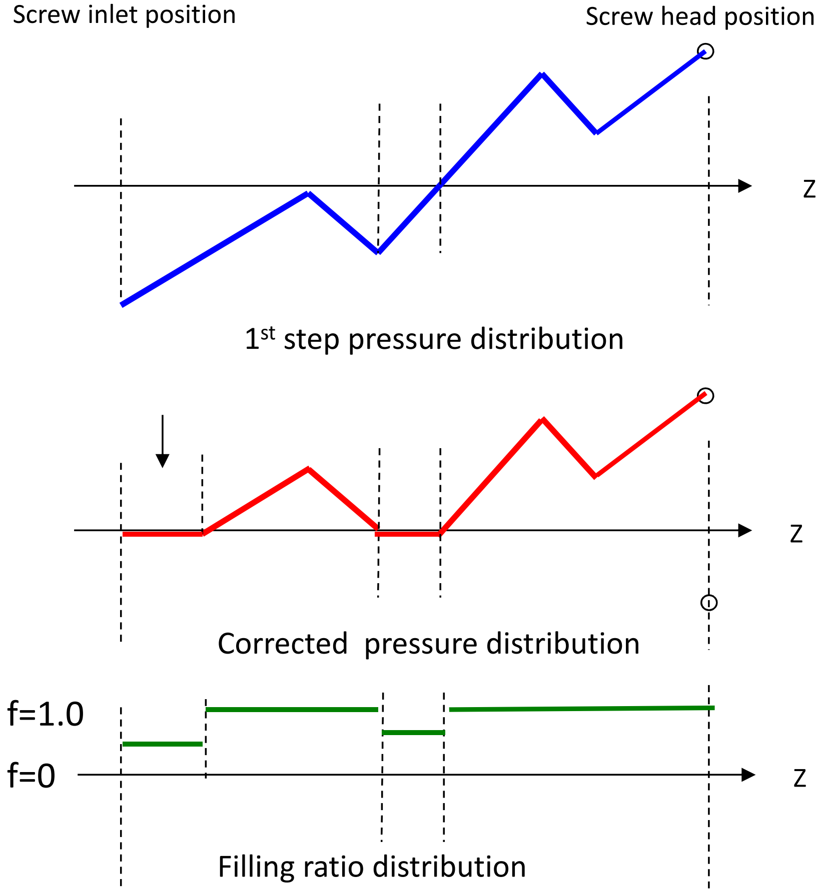
Press. at feed
0MPa（given）



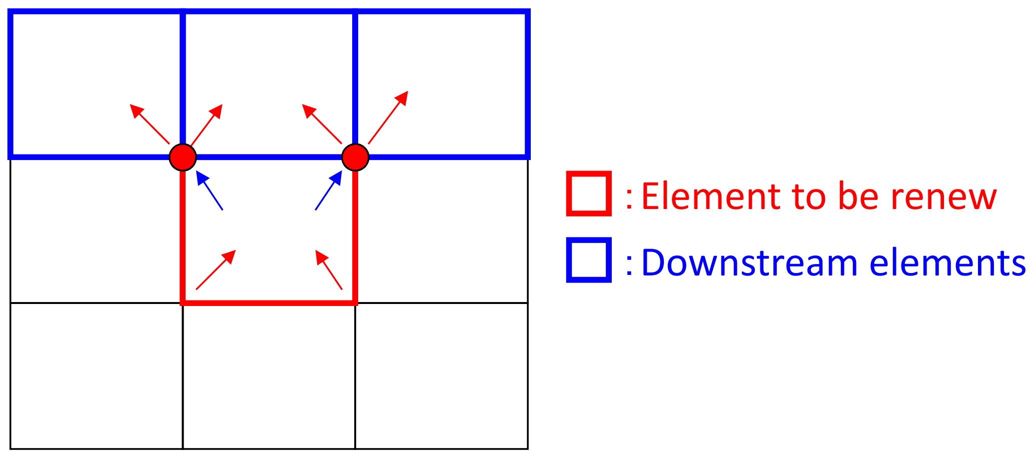
Head press.
5MPa（given）

Q = 20kg/h(given)

Pressure downstream update scheme



FAN method (1D)



Pressure downstream update scheme

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

As the pressure is need to be determined according to the two coordinates (z, θ), the pressure downstream update scheme is developed.

2.5D FEM

Criteria of filled and unfilled

Pressure gradient	Flow balance	Pressure	Fill or Unfill
$dp/dx<0$	$Q>Q_d$	$p>0$	Filled[1] $f^e=1$
$dp/dx>0$	$Q<Q_d$	$p>0$	Filled[2] $f^e=1$
$dp/dx>0$	$Q<Q_d$	$p<0 \rightarrow p=0$	Unfilled[3] $f^e=0$

1) $Q>Q_d$, unfilled state is impossible.

2) $Q<Q_d$, $p>0$: Filled sate and back flow (pressure gradient driven flow) is larger than the net flow.

3) $Q<Q_d$, $p<0$: Unfilled state and correction of $p=0, W=fW$ are applied for FAM method ($f=Q/Q_d$).

$$Q = \underbrace{\frac{WV_bH}{4}\sin(2\theta)}_{\text{Drag-force driven flow } Q_d} - \underbrace{\frac{WH^3}{12\eta}\left(\frac{dp}{dx}\right)}_{\text{Pressure gradient driven flow, } Q_p}$$

Correction of pressure distribution

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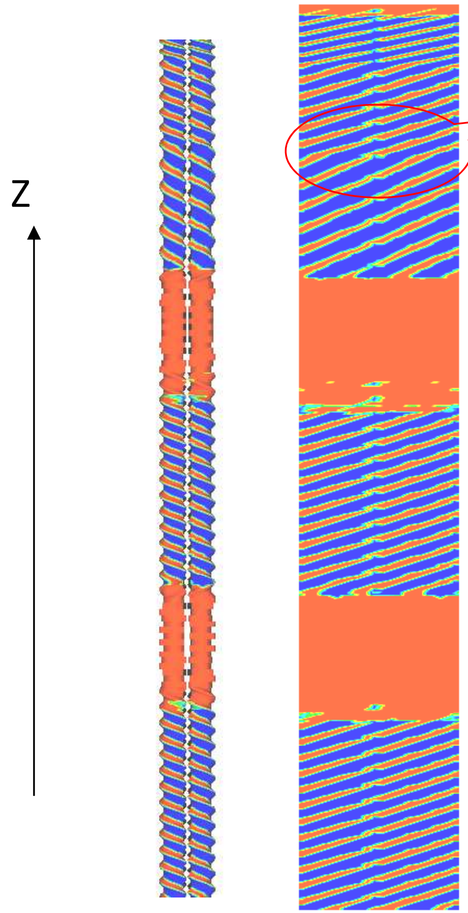
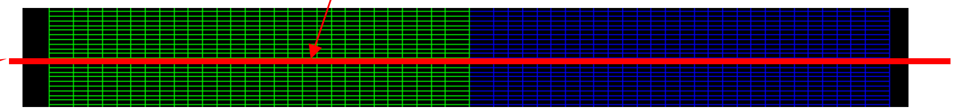


Fill ratio control line



$\uparrow Q_{ext}$

Average fill ratio determined by pressure distribution

$$f^{av} = \frac{\sum V^e f^e}{\sum V^e}$$

z-axis fill ratio determined by screw geometry

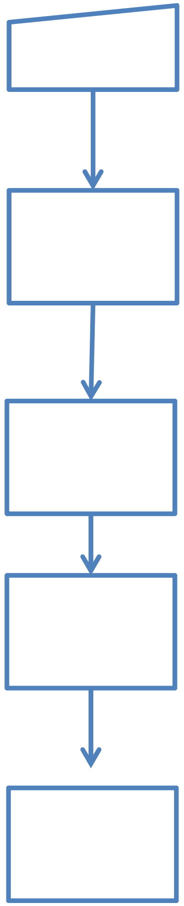
$$Q_d^z = V_d^{ave} \cos\phi \sin\phi \Delta X H$$

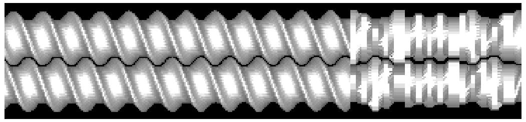
$$= \sum_{D_\alpha} D_\alpha \left(\frac{\Delta X}{\Delta Z} \sin\phi \cos\phi \right)$$

$$f^z = \frac{Q_{ext}}{\sum Q_d^z}$$

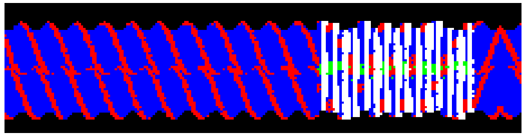
Adjusting pressure distribution to agree f^{av} with f^z.

Performing simulation

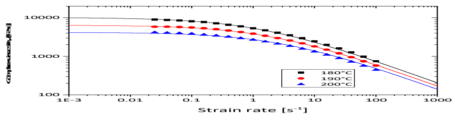




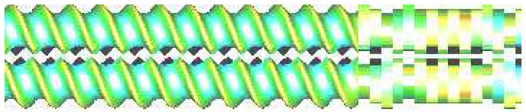
Simple wizard for constructing screw geometry



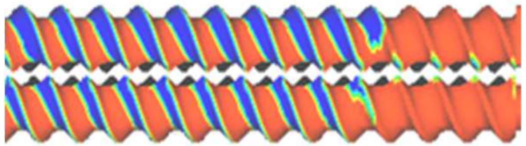
Automatic meshing



Viscosity-strain rate model e.g., Cross model
Operation variables (Feed rate, Q, Head pressure P, Rot speed N)

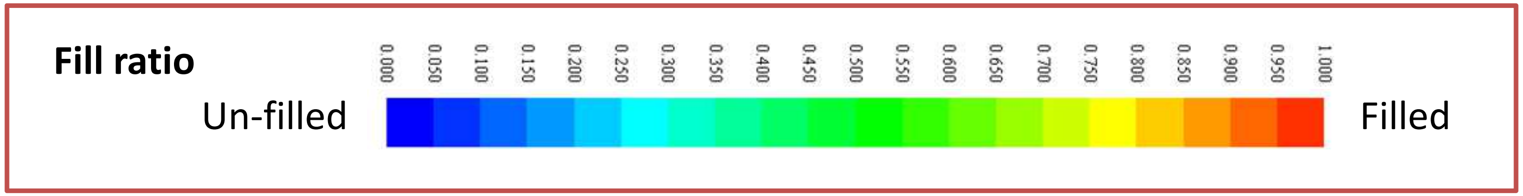


Calculation of pressure distribution by FEM.

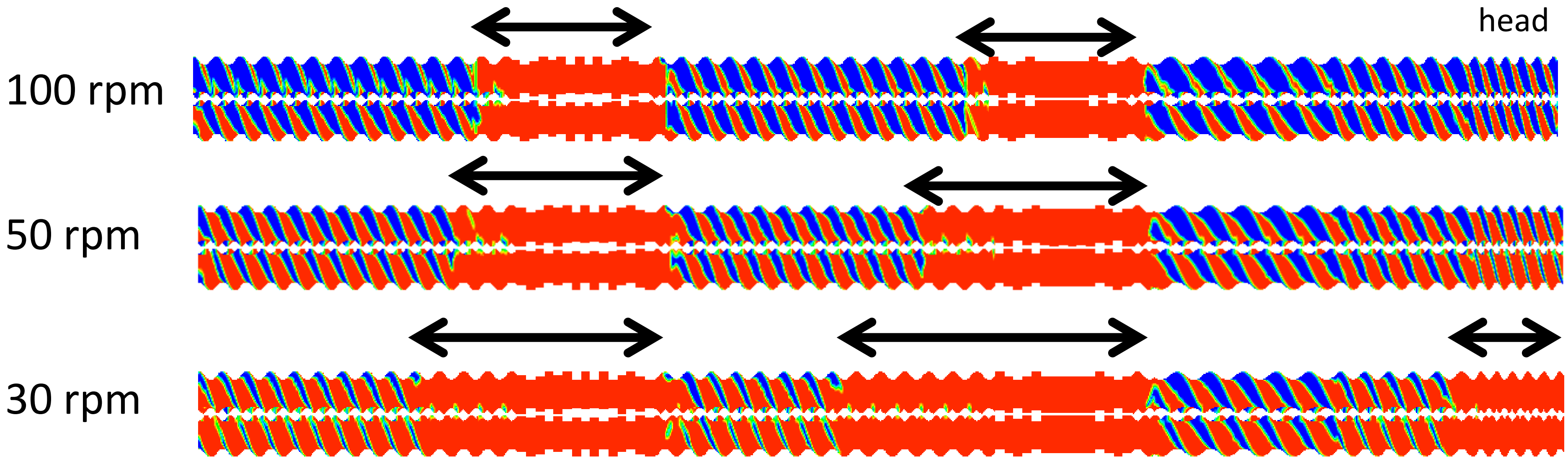


Fill ratio distribution

Effect of Screw Speed (rpm)

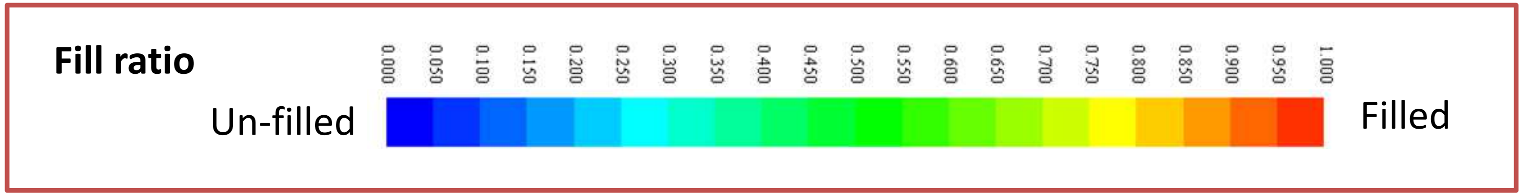


Feed rate 0.75kg/h



Decrease of screw speed expands filled region backwards.

Effect of feed rate (kg/h)

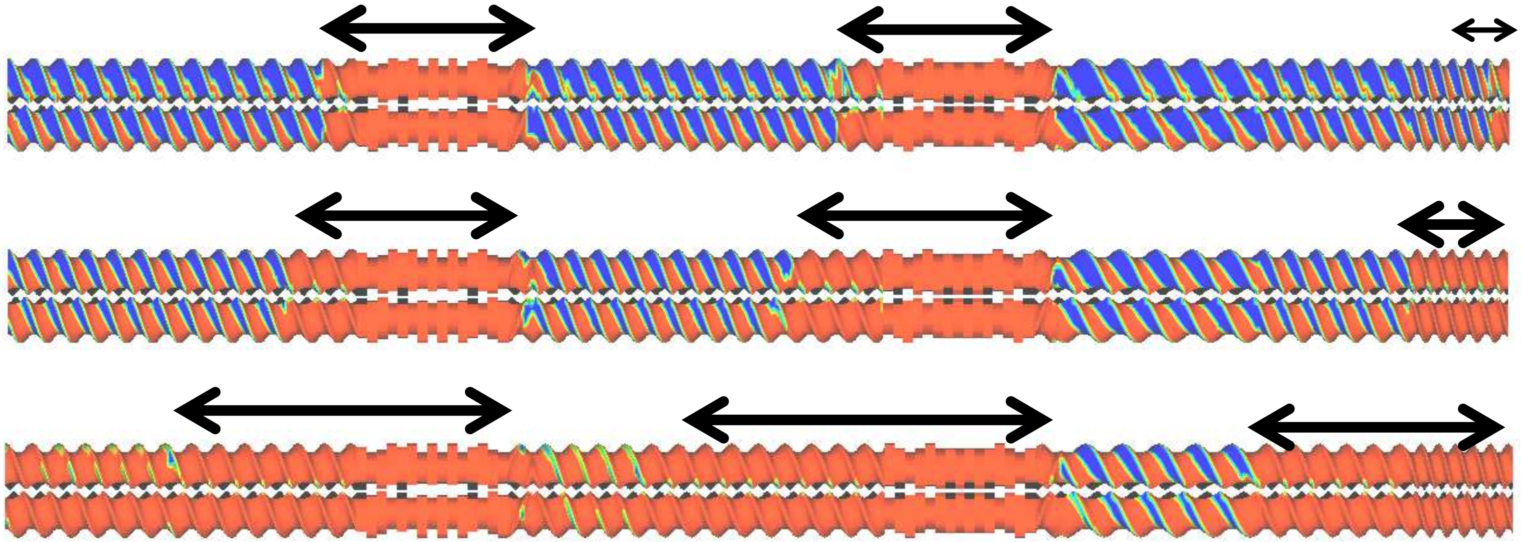


Speed 30 rpm

0.25 kg/h

0.50 kg/h

0.75 kg/h



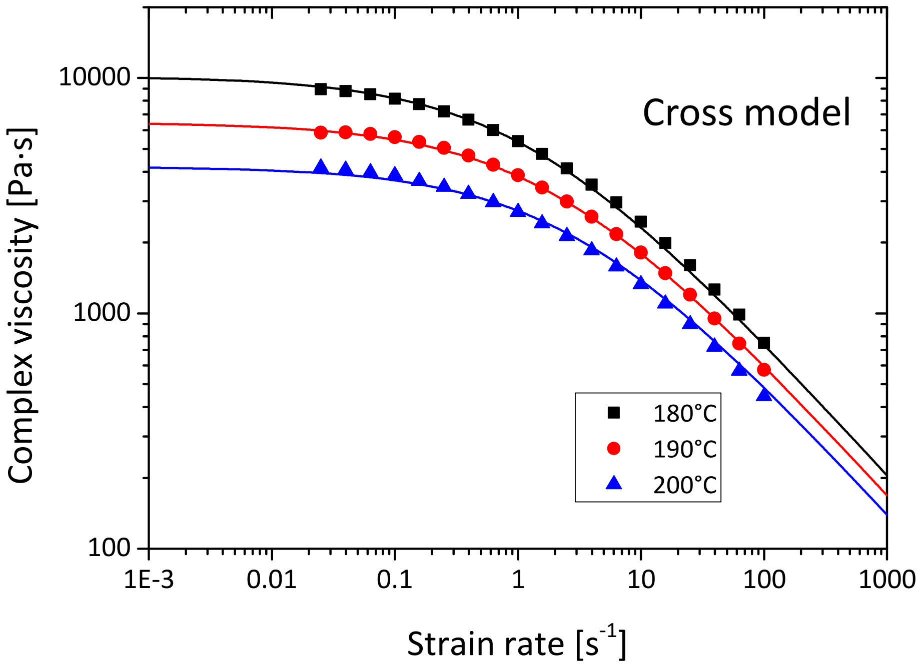
Increase of feed rate expands filled region backwards.

Experiments

Material

Homo polypropylene (F-704NP, Prime Polymer, Japan)

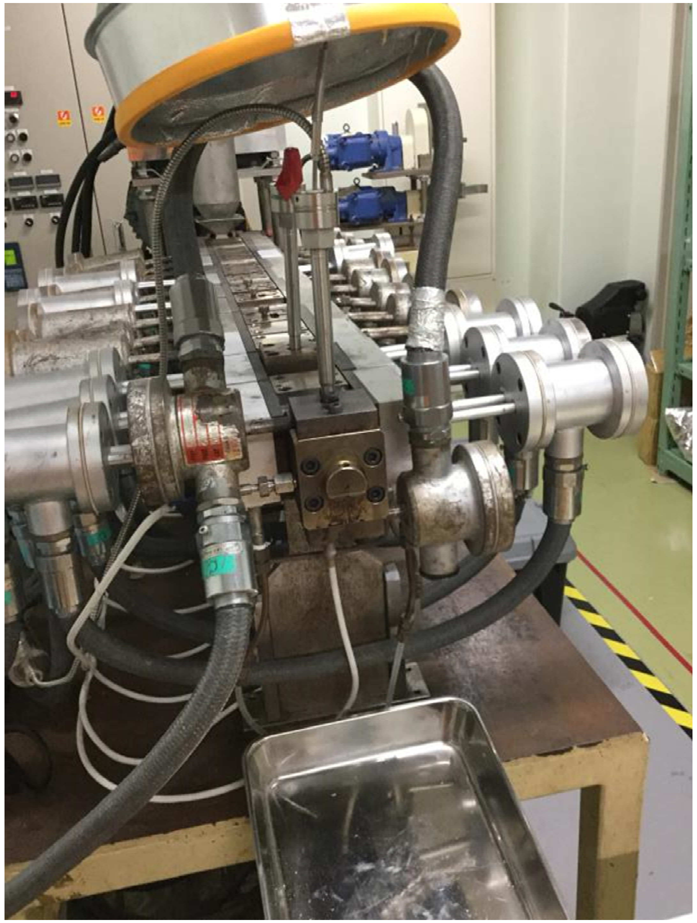
Viscosity-strain rate curve was obtained by the Cross model



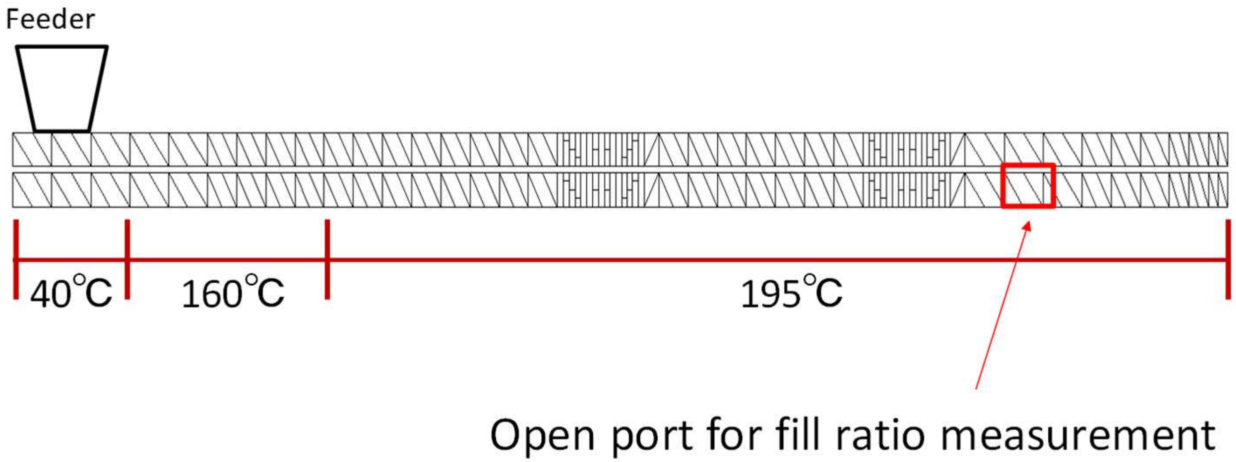
$$\eta(\dot{\gamma}, T, P) = \frac{\eta_0}{1+\left(\frac{\eta_0 \dot{\gamma}}{\tau^*}\right)^{1-c}}$$

$$\eta_0 = a \exp\left(\frac{T_b}{T+273.15}\right)$$

Screw geometry and barrel temp.



Self-wiping co-rotating parallel twin screw extruder
L/D = 90, ϕ = 15 mm
(Technovel, Japan)



Fill ratio distribution

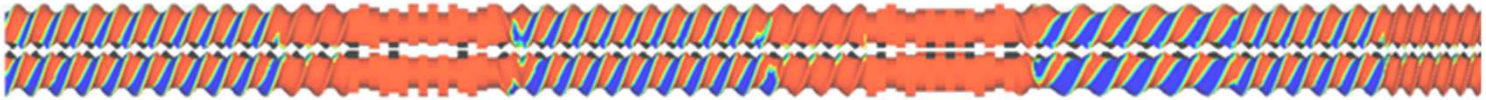
30 rpm
0.5 kg/h

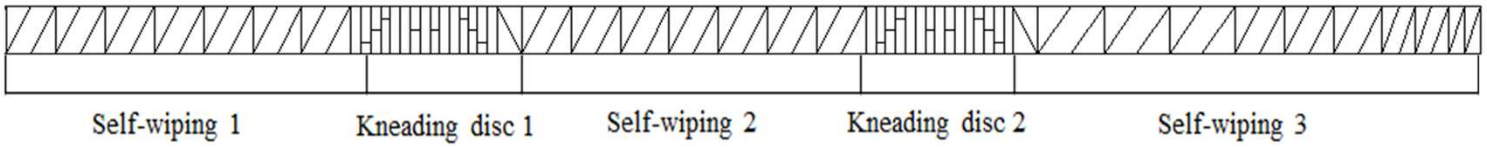
Fill ratio

Low (0)  High (1)

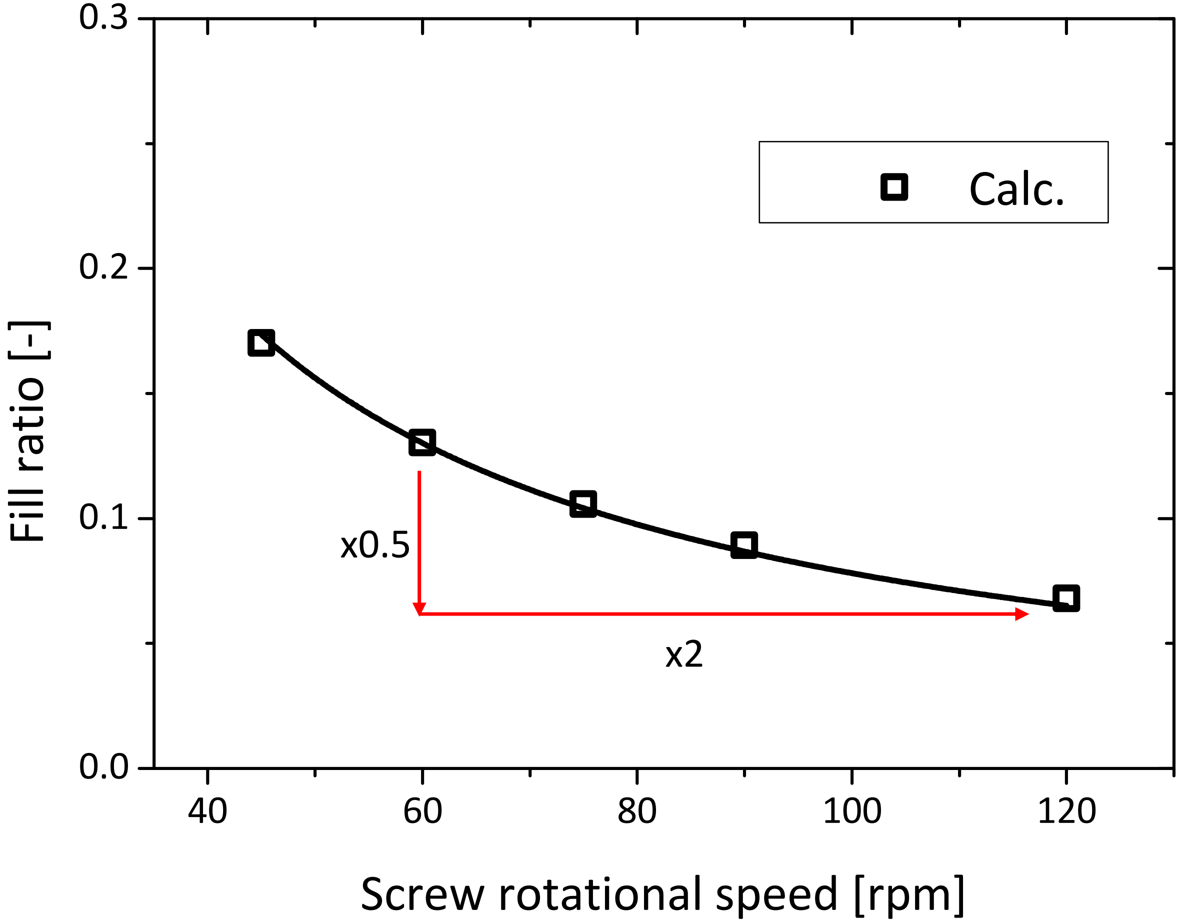
Pulled-out screw

Simulation



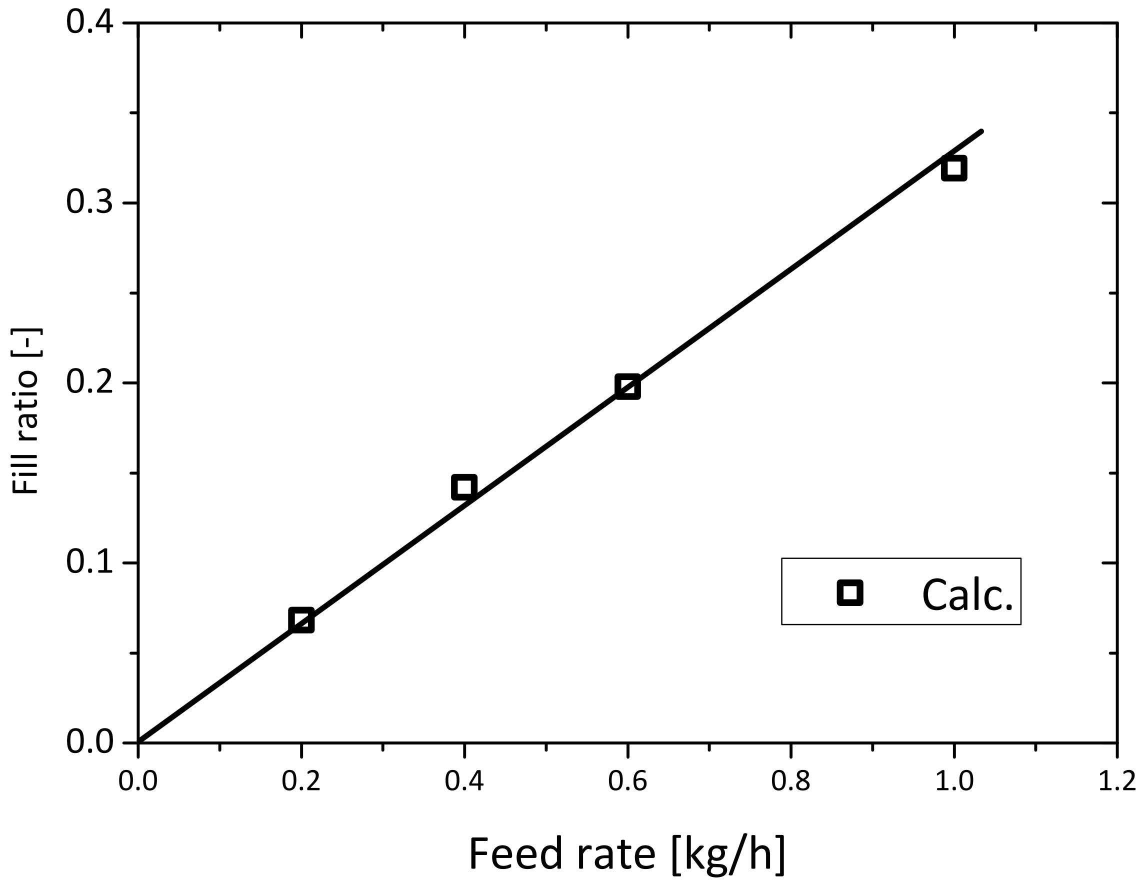


Screw speed (rpm) vs. Fill ratio



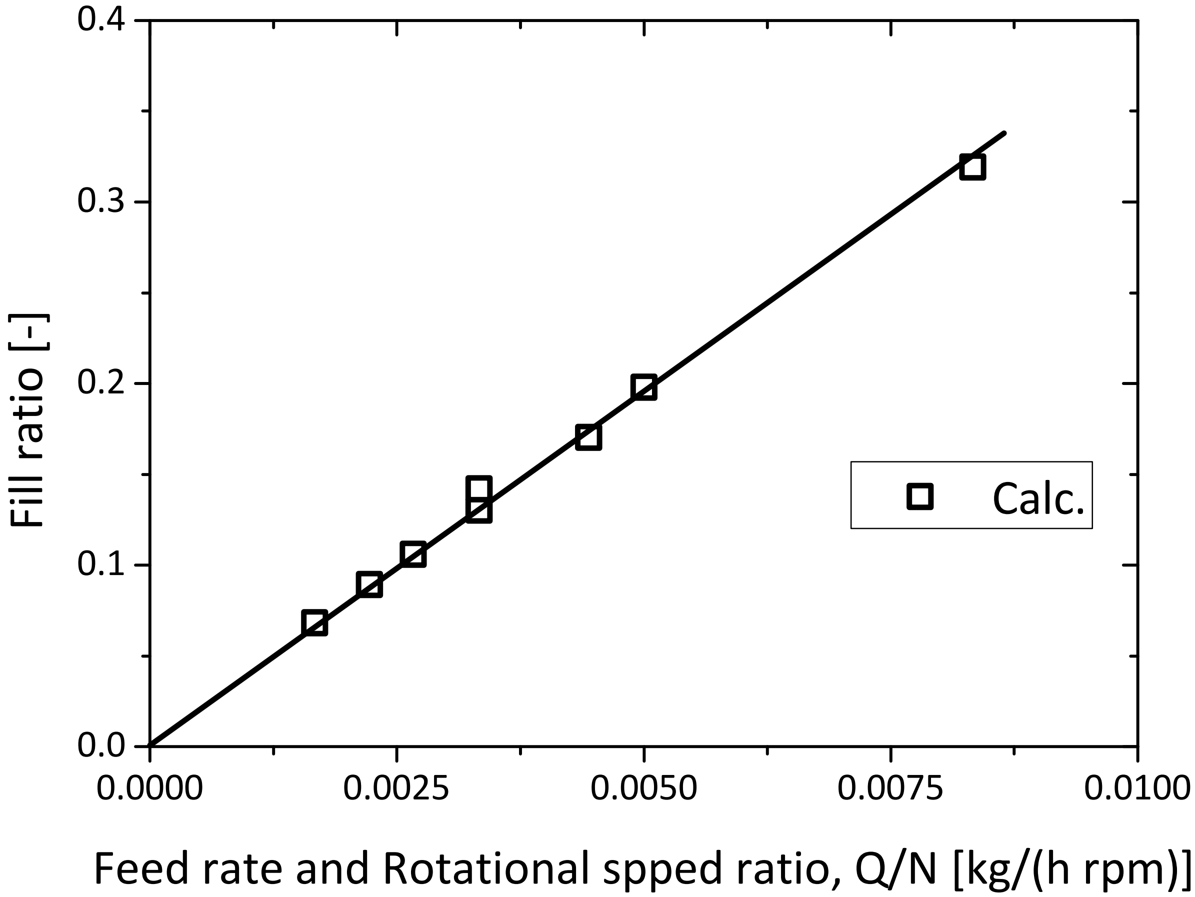
The calculation results agree with the theoretical definition, Q/Q_d as the fill ratio became half when the screw speed becomes double.

Feed rate vs. fill ratio



Calculation agrees with the theoretical definition of fill ratio, Q/Q_d as the plots exist on the straight line from origin.

Throughput vs. fill ratio



Calculation agrees with the theoretical definition of fill ratio, Q/Q_d as the plots exist on the straight line from origin.

Conclusion

- We achieved a development of 2.5D Hele-Shaw model for calculation of pressure distribution in twin screw extruder.
- This model has advantage for short-calculation time, possible to whole screw elements.
- The fill ratio was calculated based on the FAN method.
- Further experimental validations not only the fill ratio but also fiber attrition, plasticization etc are demanded.
- Devolatilization model will be added.

Contact information

- This software is proprietary and commercially available by the HASL Co. ltd., Japan.
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Thank you for your kind attention.