“Mathematical modeling of the twin screw Extrusion Processing of Energetic Materials for Tangential vs fully-intermeshing and co vs counter-rotating”

Joint Ordnance Commanders Group (JOCG)
Continuous Mixer & Extruder Users Group (CMEUG)
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Stevens Institute of Technology

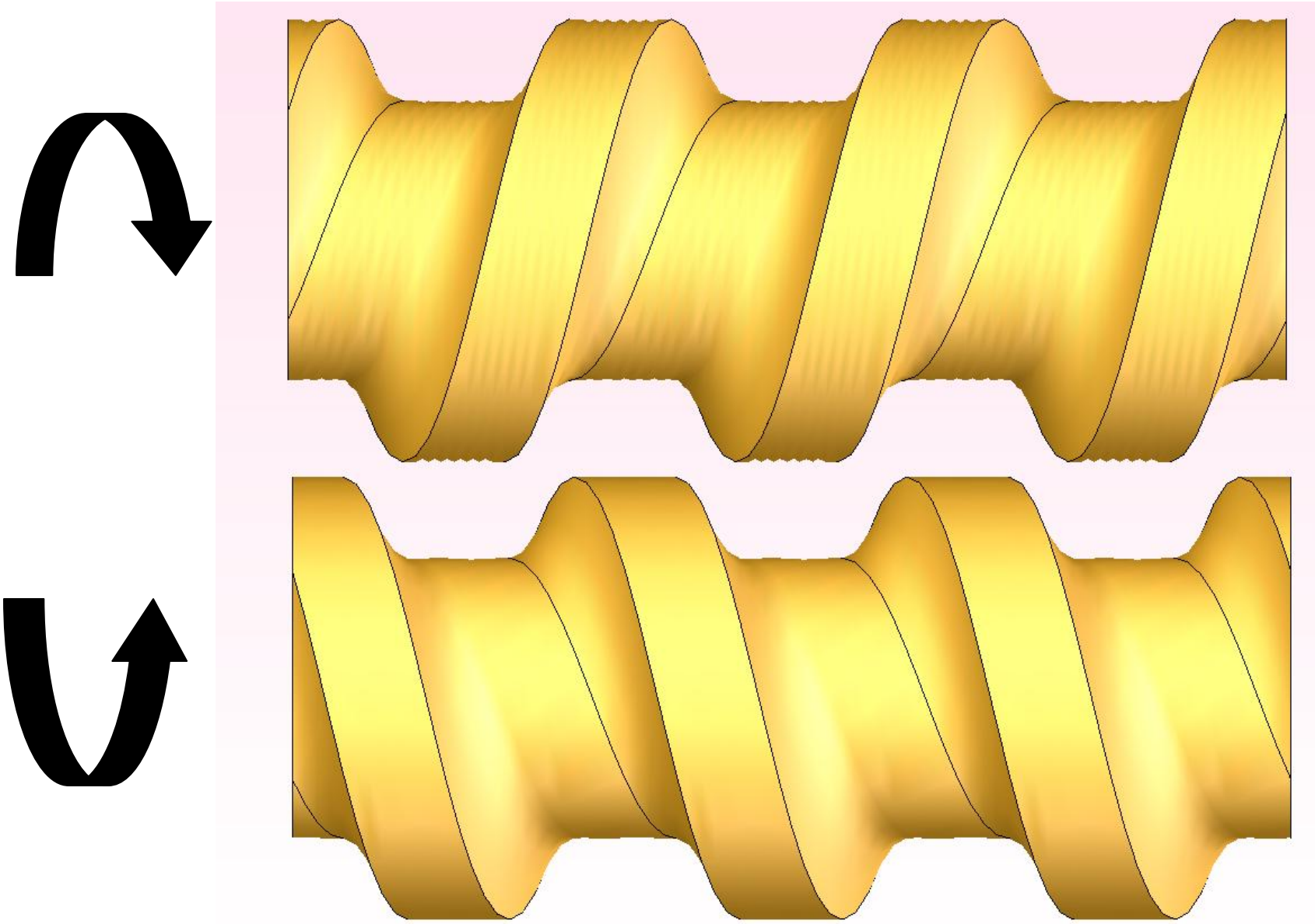
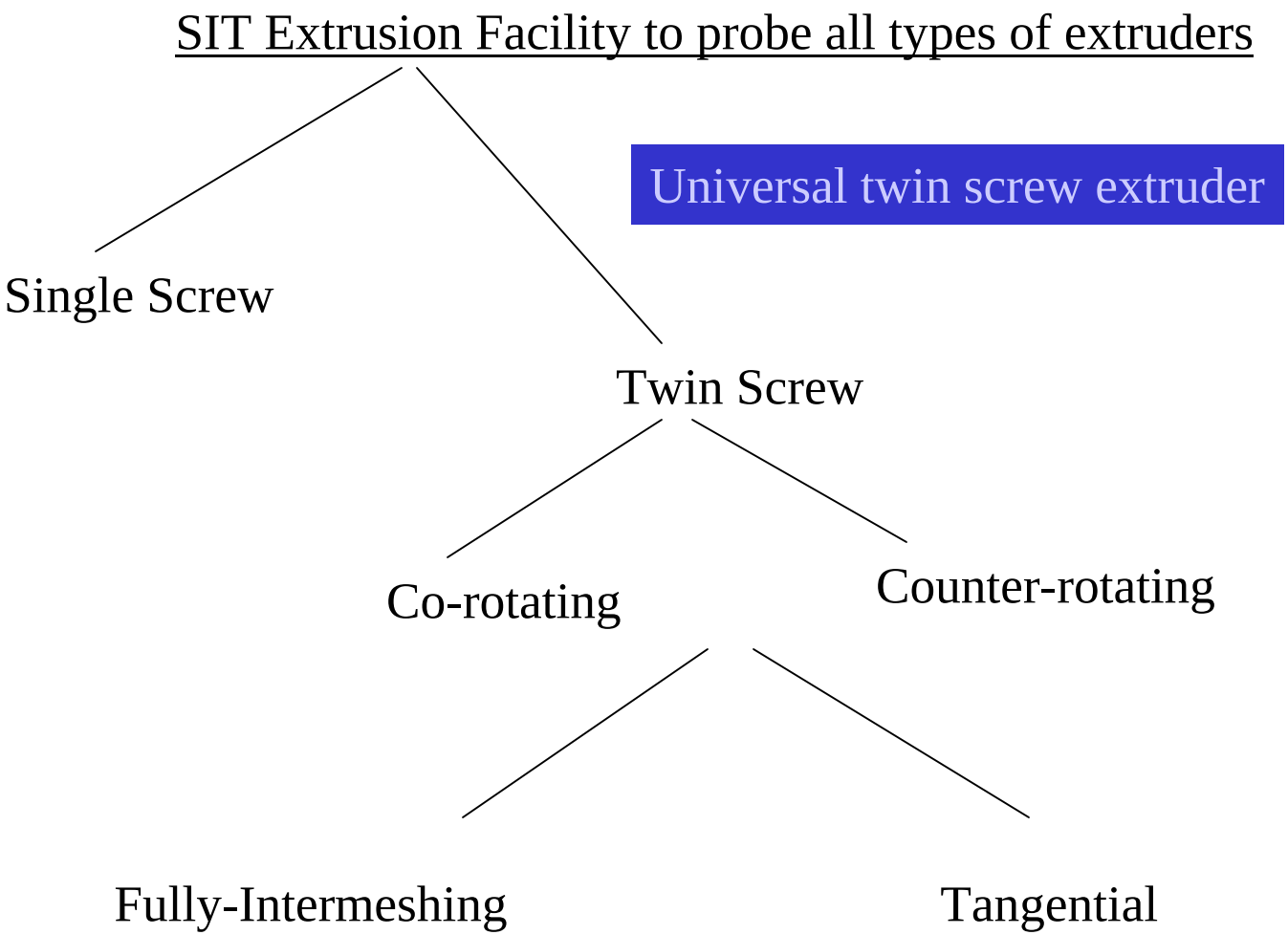
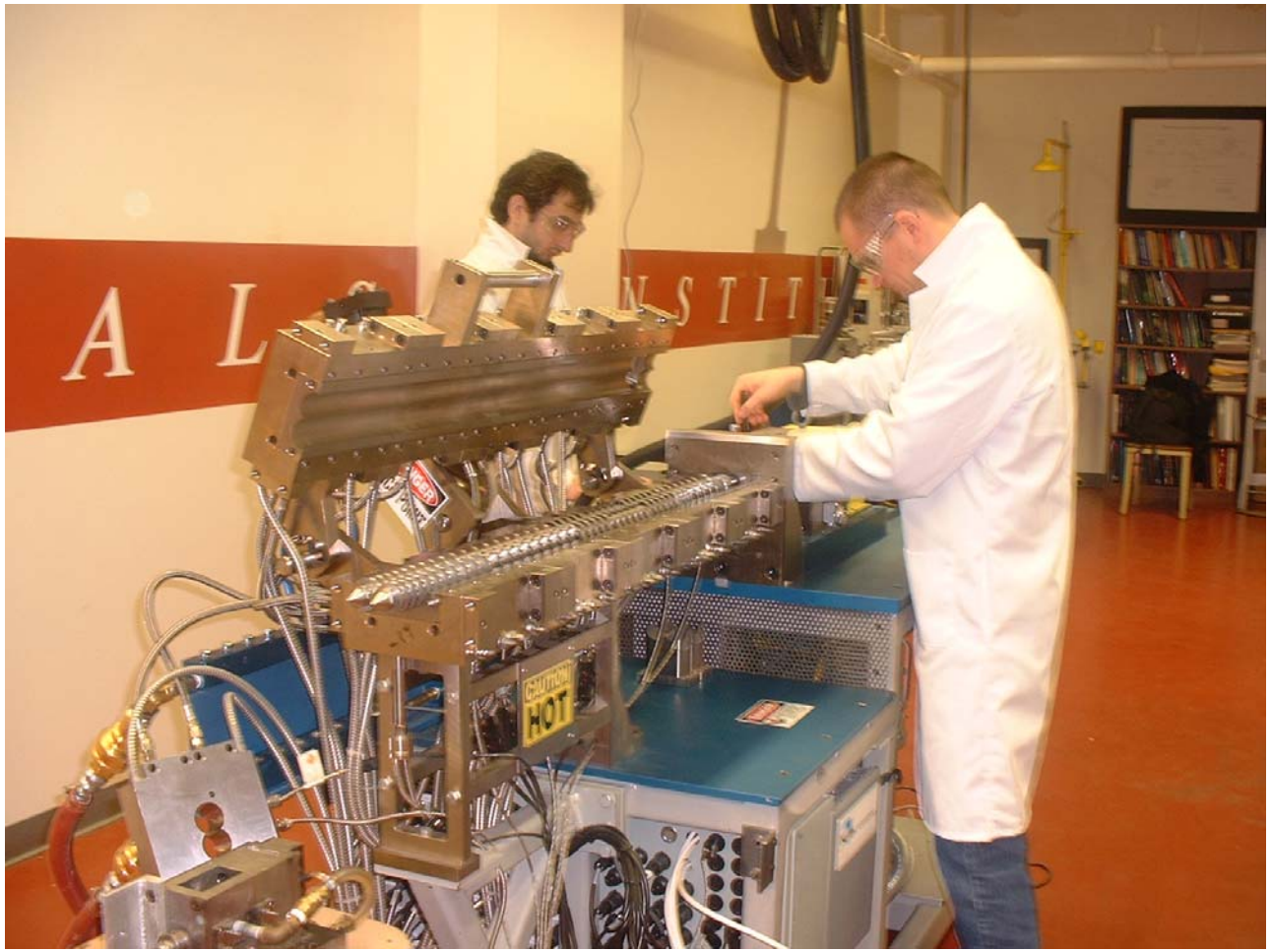


Fig.7c. Counter-rotating tangential twin screws.


SIT Extrusion Facility to probe all types of extruders
Universal twin screw extruder
Single Screw
Twin Screw
Co-rotating
Counter-rotating
Fully-Intermeshing
Tangential

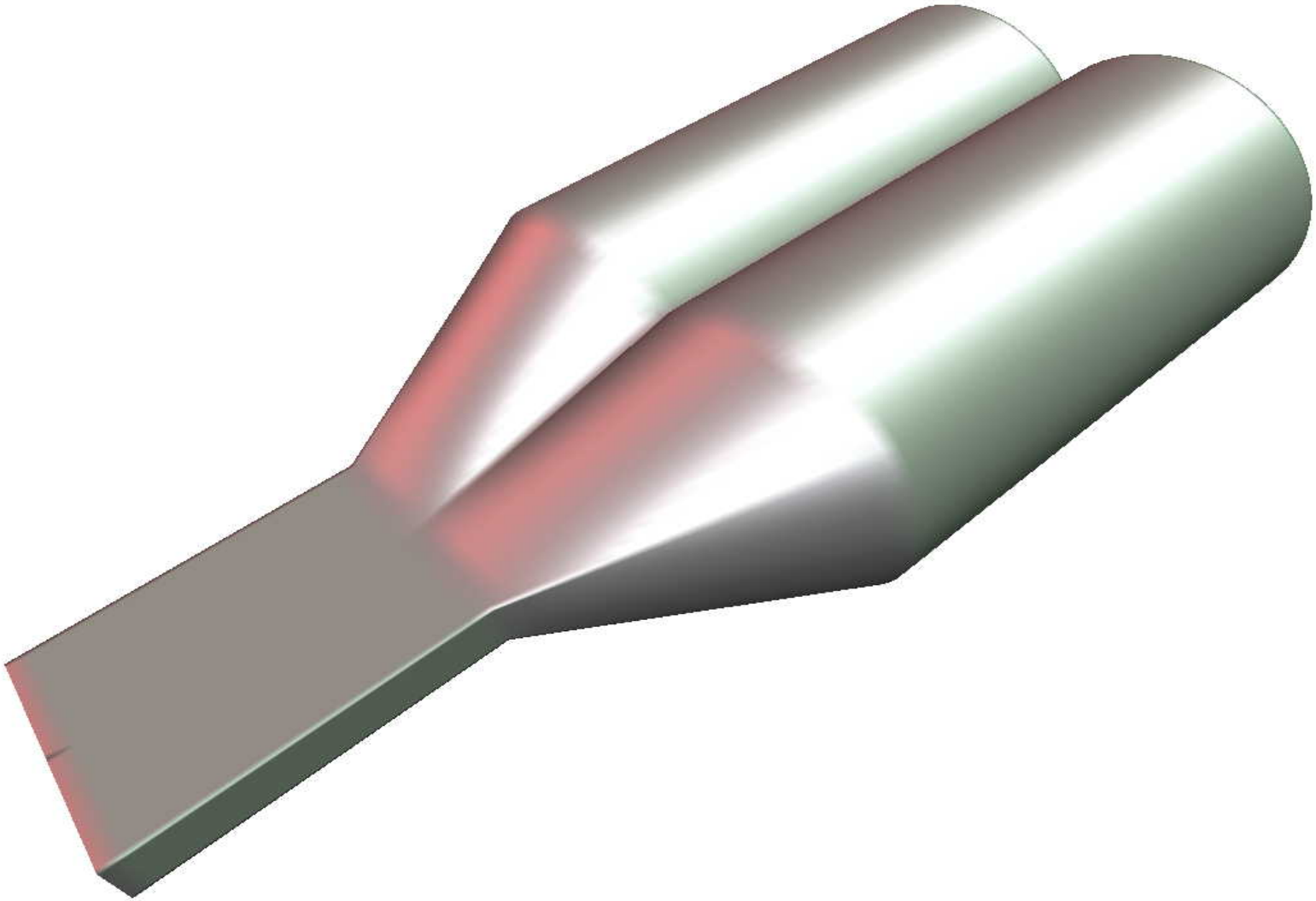


Universal twin screw extruder

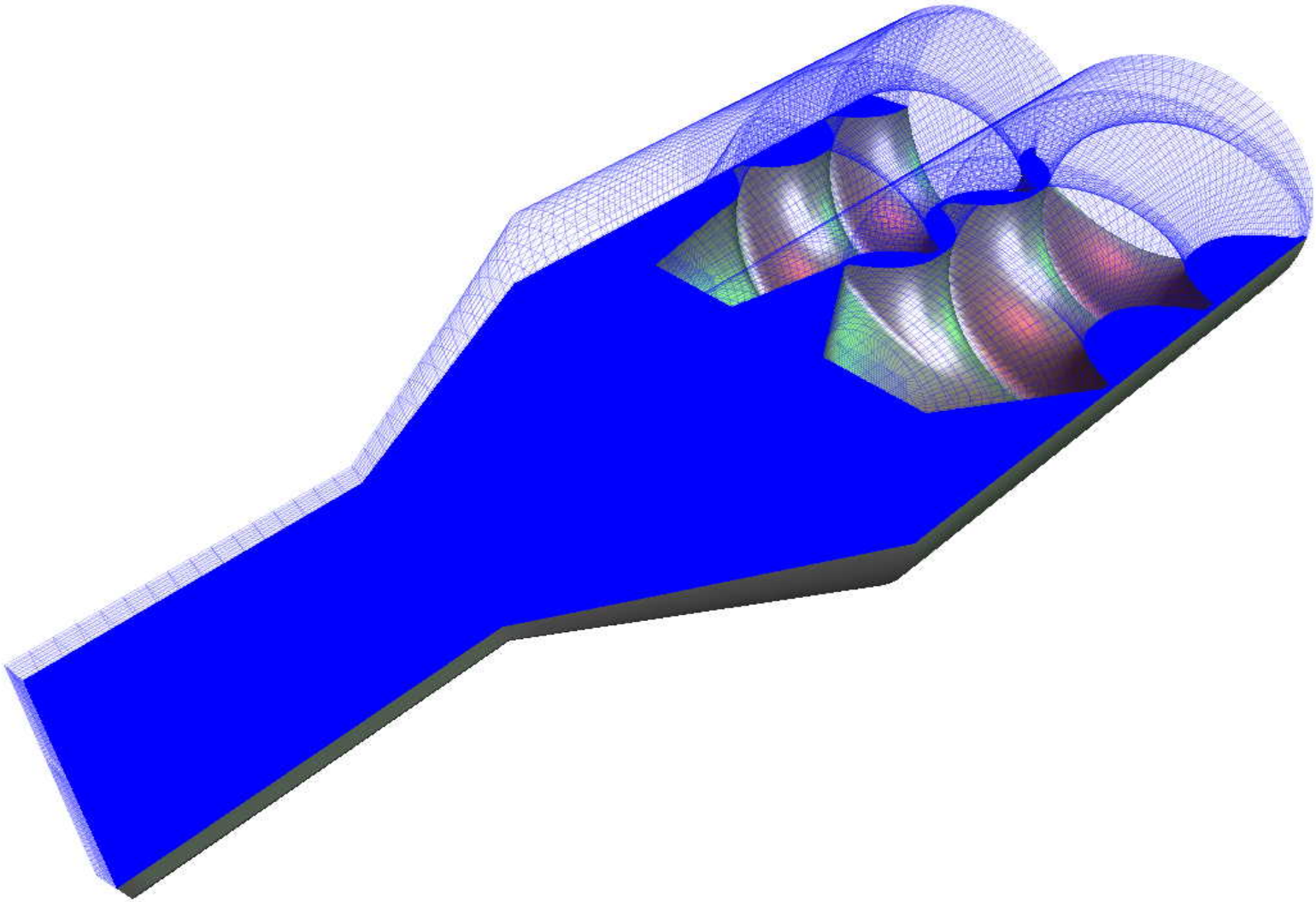
Mathematical modeling

- Up to this point our simulations were carried out on the fully-intermeshing co-rotating twin screw extrusion
- There are a number of advantages to using other types of extruders depending on the task at hand
- Are the simulation technologies equally applicable to other types of extrusion
- Use the coupled die and extrusion flow as a realistic combination to probe.

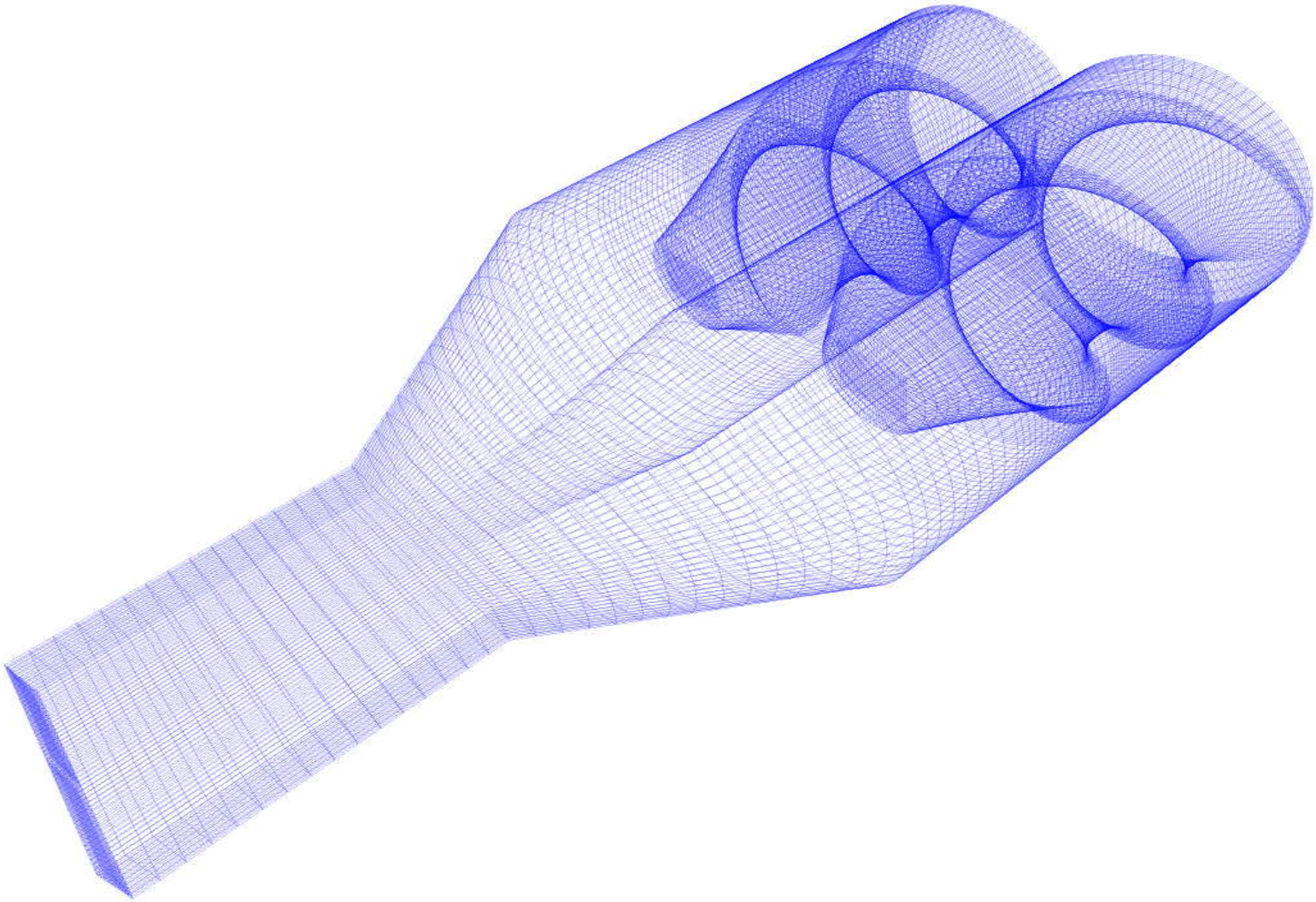
Co-rotating Fully-Intermeshing Twin Screw Extrusion



Flow Channel Solid Model



Flow Channel Cutaway



FEM Mesh

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} = 0$$

$$Q - \int_D u_z dD = 0$$

Realistic channel, GNF

$$\frac{\partial p}{\partial x} = \frac{\partial}{\partial x}\left(2\eta\frac{\partial u_x}{\partial x}\right) + \frac{\partial}{\partial y}\left[\eta\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)\right]$$

$$\frac{\partial p}{\partial y} = \frac{\partial}{\partial y}\left(2\eta\frac{\partial u_y}{\partial y}\right) + \frac{\partial}{\partial x}\left[\eta\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)\right]$$

$$\frac{dp}{dz} = \frac{\partial}{\partial x}\left(\eta\frac{\partial u_z}{\partial x}\right) + \frac{\partial}{\partial y}\left(\eta\frac{\partial u_z}{\partial y}\right)$$

$$Pe\left(u_x \frac{\partial\theta}{\partial x} + u_y \frac{\partial\theta}{\partial y} + u_z \frac{\partial\theta}{\partial z}\right) = \left(\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2}\right)$$

$$+ \quad G \quad \eta \quad (|\dot{\gamma}|)^2$$

$\Theta=(T-T_o)/(T_b-T_o)$
T_b (Barrel Temperature) ; T_o (Entrance Temperature)

1. **at z=0 (Entrance) $\Theta=0$**
2. **On the barrel surface $\Theta=1$**
3. **On the screw surface** $\frac{\partial\theta}{\partial \underline{n}} = 0$

Conservation of linear momentum upon application of Bubnov Galerkin:

$$\int_D \nabla\pi \cdot \underline{\underline{T}}\, dD - \int_{\Gamma_s} \pi(\underline{n}\,\underline{t} : \underline{\underline{T}})\underline{t}\, d\Gamma_s - \int_{\Gamma_s} \pi(\underline{n}\,\underline{n} : \underline{\underline{T}})\underline{n}\, d\Gamma_s = 0$$

Weighting function

Total stress tensor

Unit tangent vector

Unit normal vector

$$\underline{t} \cdot (\underline{u} - \underline{u}_{solid}) = \beta \underline{n}\,\underline{t} : \underline{\underline{T}}$$

Wall slip

Navier's slip coefficient

$$\underline{n} \cdot (\underline{u} - \underline{u}_{solid}) = 0$$

No material exchange

Streamline Upwind Petrov-Galerkin Method (SUPG)

$$\int_z^{z+\Delta z}\left\{\int_D\left[\overline{W}^f \mathrm{Pe}\left(u_x\frac{\partial\theta}{\partial x}+u_y\frac{\partial\theta}{\partial y}+u_z\frac{\partial\theta}{\partial z}\right)\right.\right.$$

$$\left.+\nabla\overline{W}^f\cdot\nabla\theta-\overline{W}^f G\eta(|\dot{\gamma}|)^2\right]dD$$

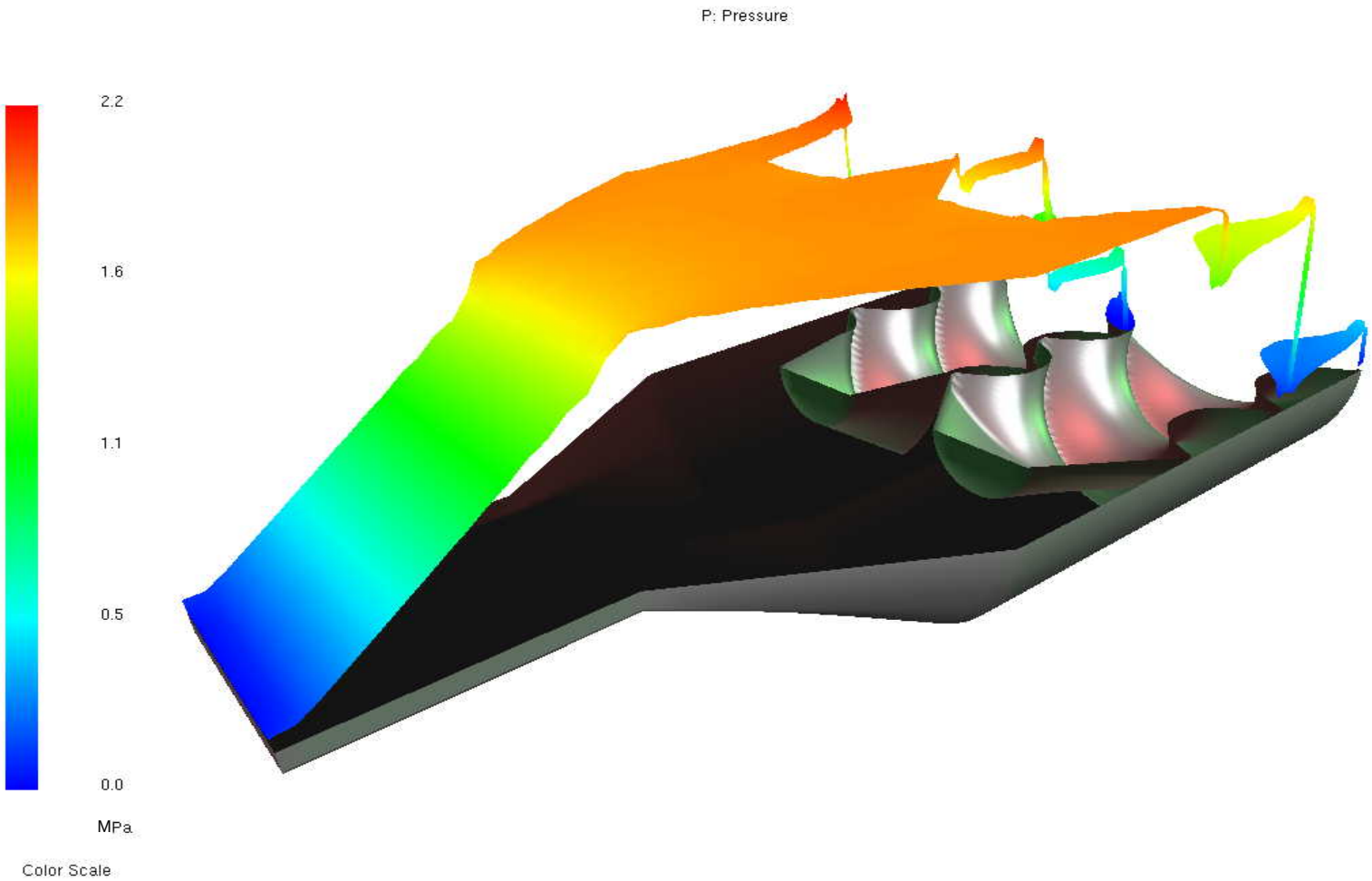
$$\left.-\int_{\Gamma_s}\overline{W}^f(\nabla\theta\cdot\underline{n})d\Gamma_s\right\}dz=0$$

Hughes et al., 86

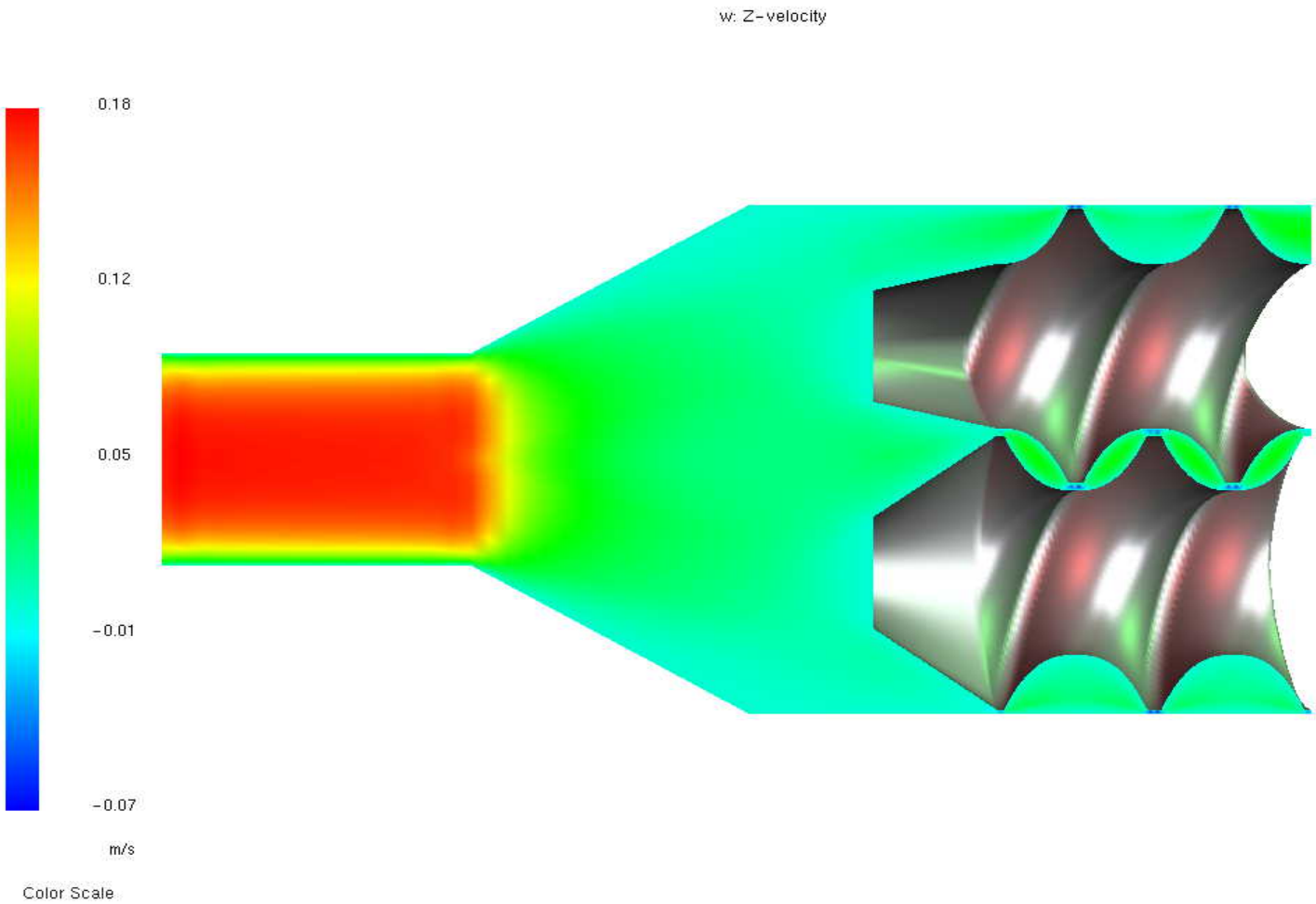
$$\overline{W}^f = W^f + w^f \qquad w^f = \frac{\sigma h^e \varepsilon^e}{2\|\underline{u}\|}\underline{u}\cdot\nabla W^f$$

$$\varepsilon^e = \coth\gamma^e - \frac{1}{\gamma^e} \qquad \gamma^e = \mathrm{Pe}\|\underline{u}\|h^e/2$$

$$h^e = 2\|\underline{u}\|/b$$



1 lead, 100 RPM, 230 lb/hr, 180°C, P_{max} = 279 psi, m = 10,000 Pa-s^n, n = 0.5



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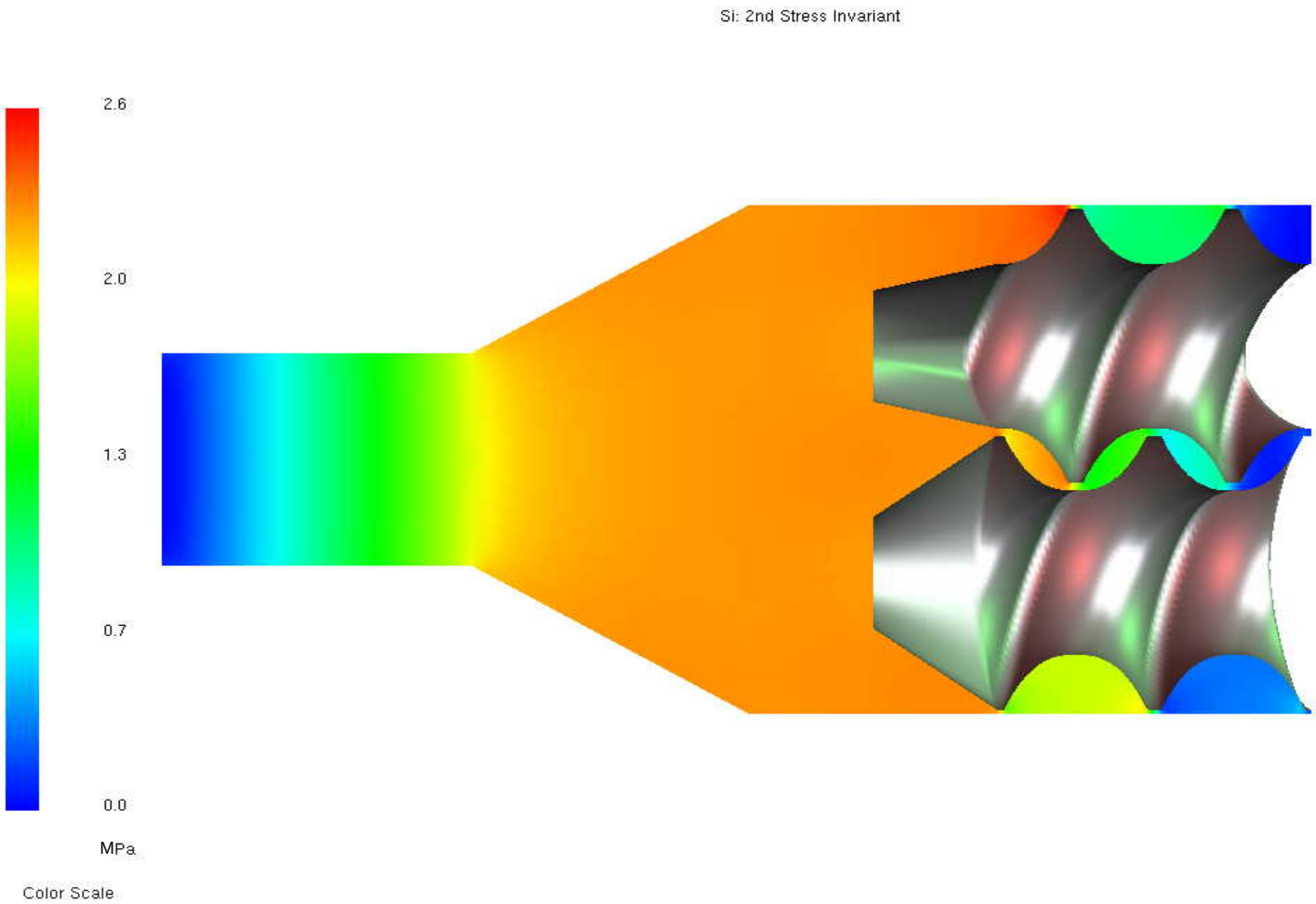

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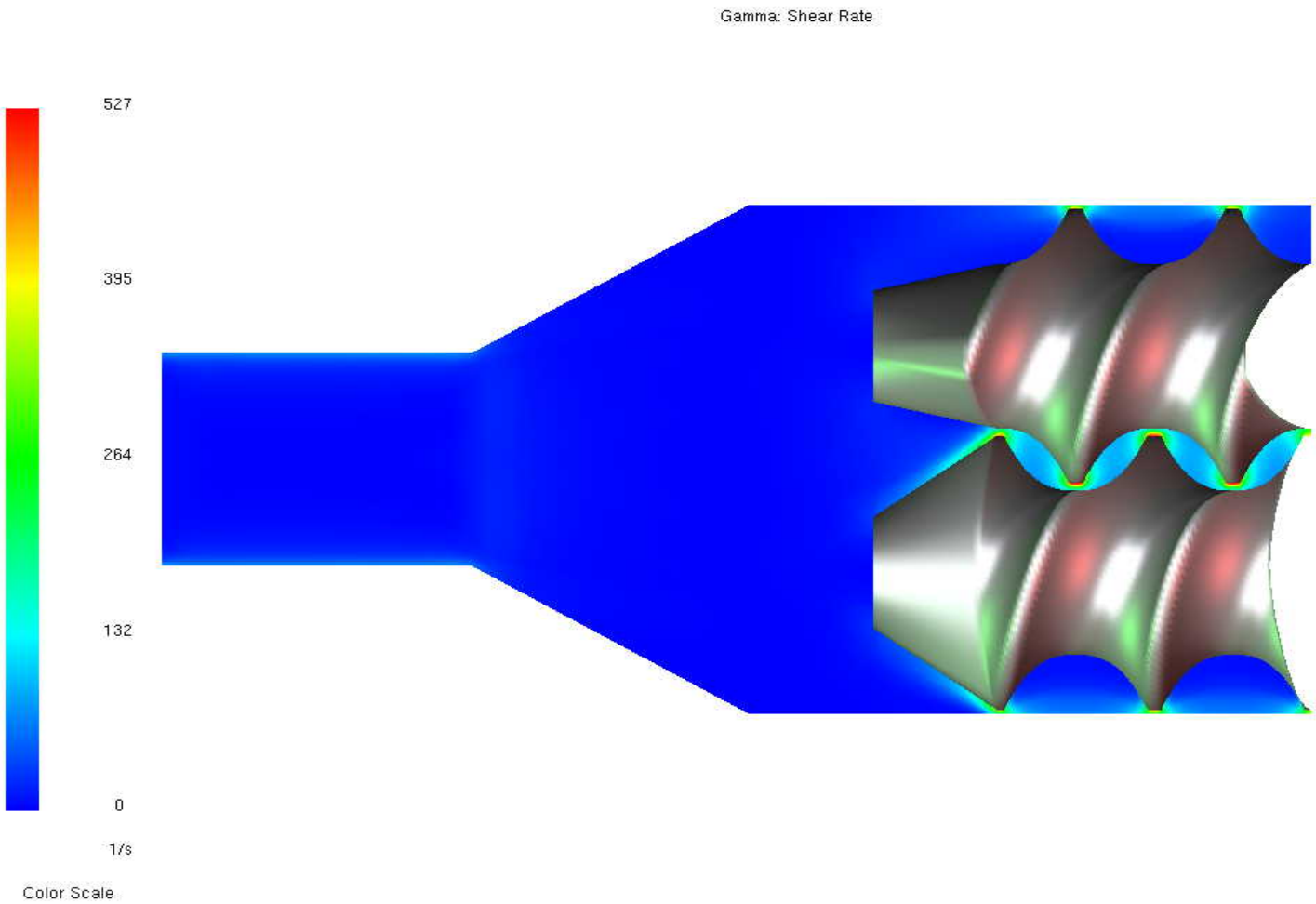

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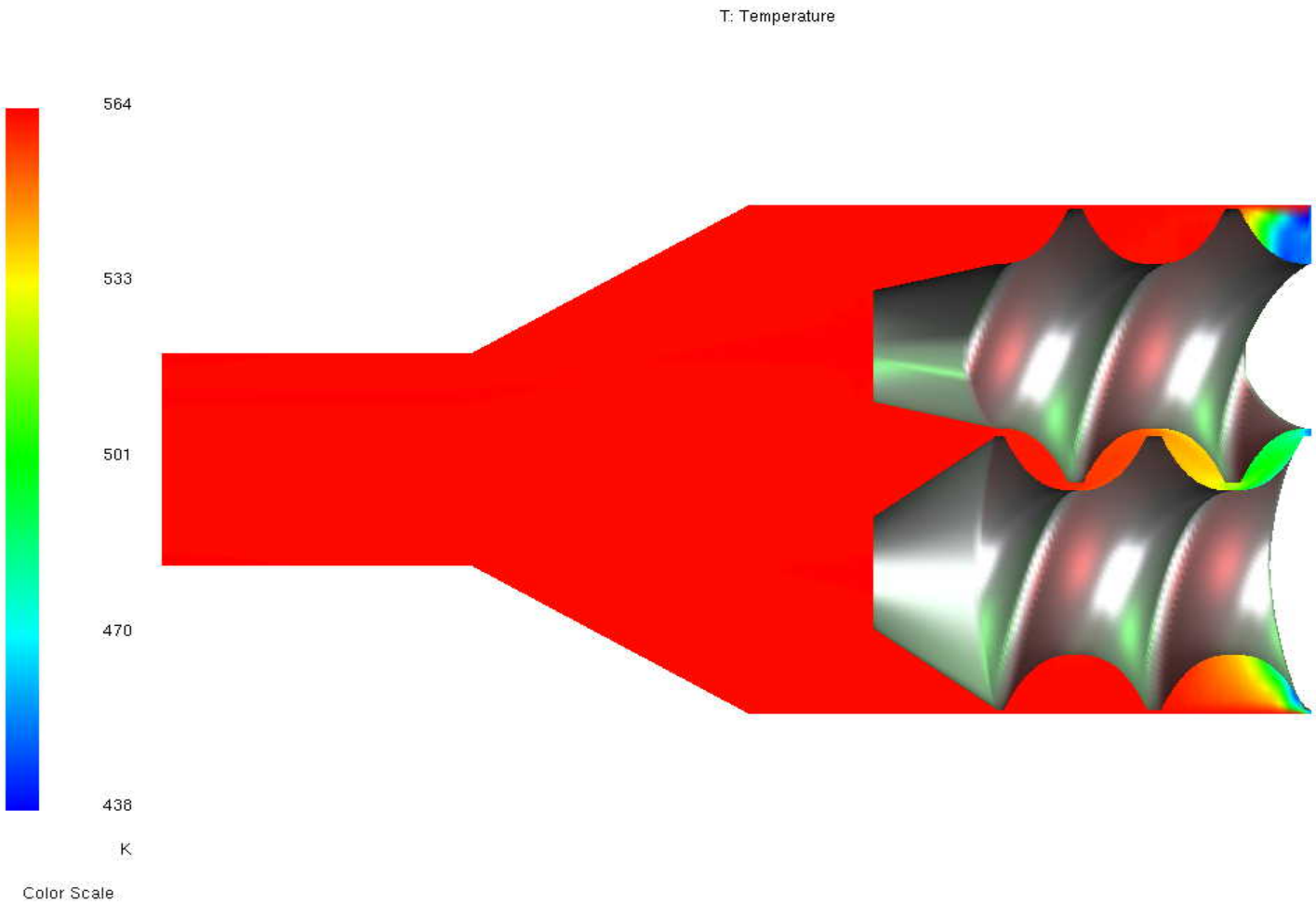

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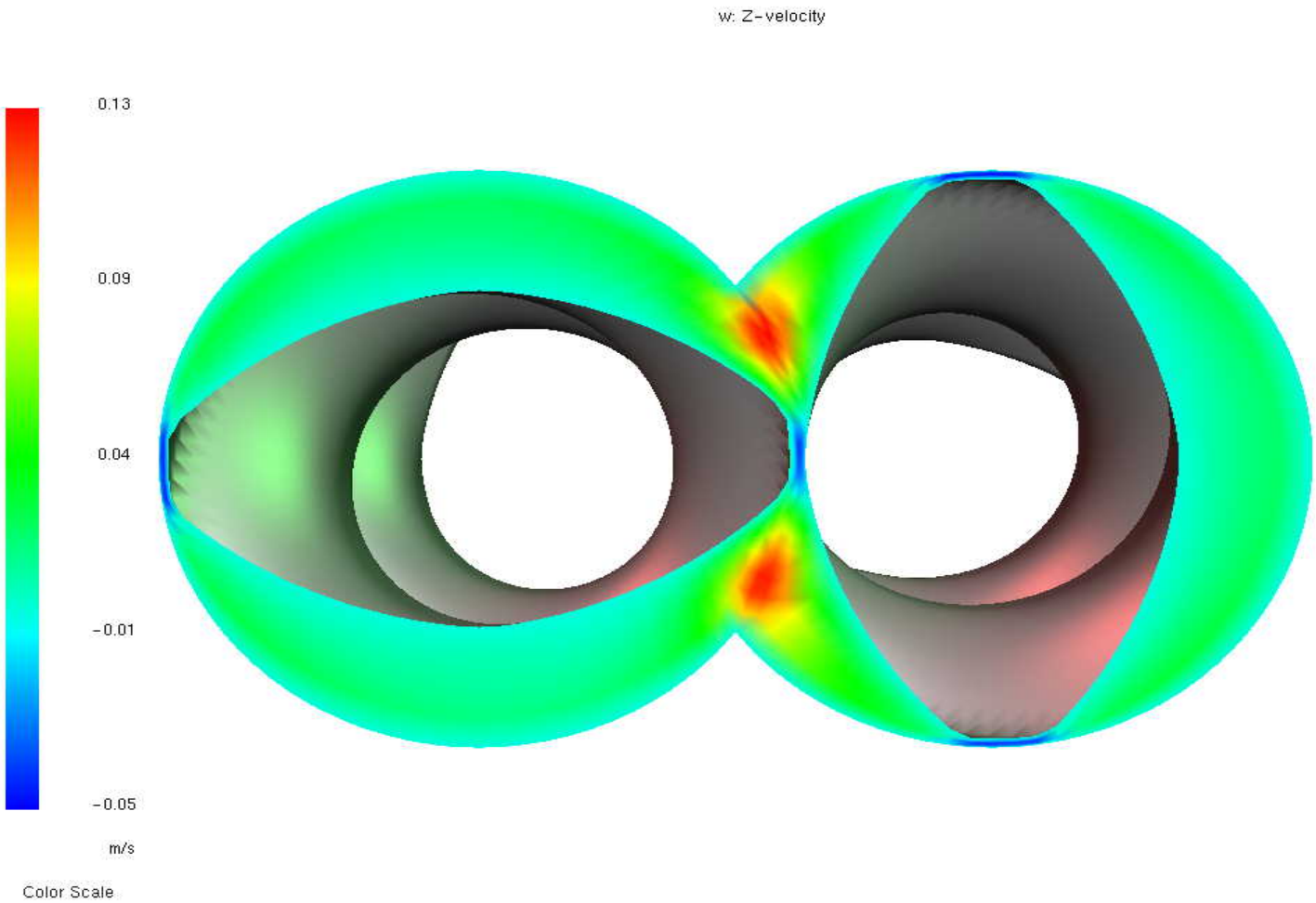

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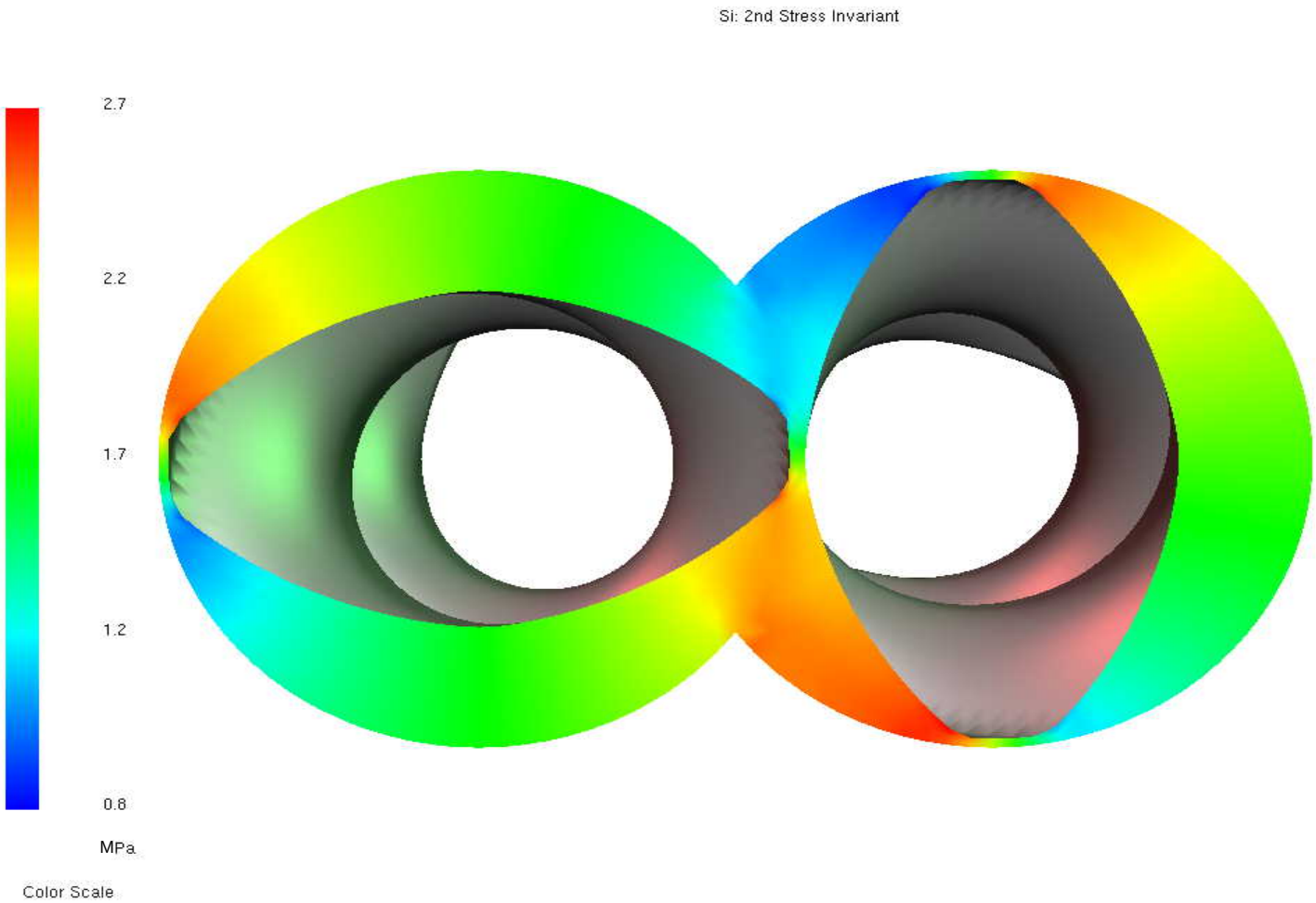

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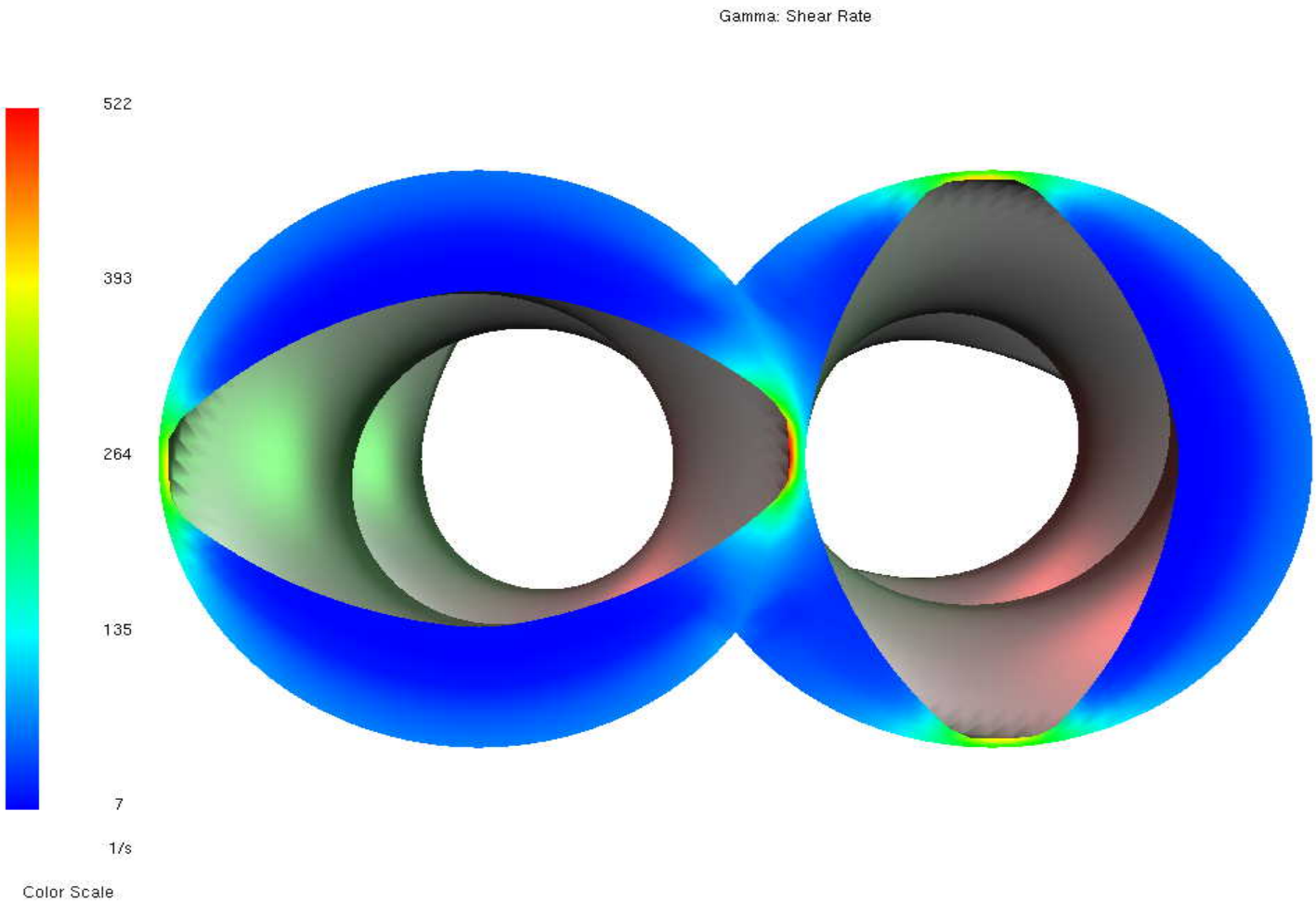

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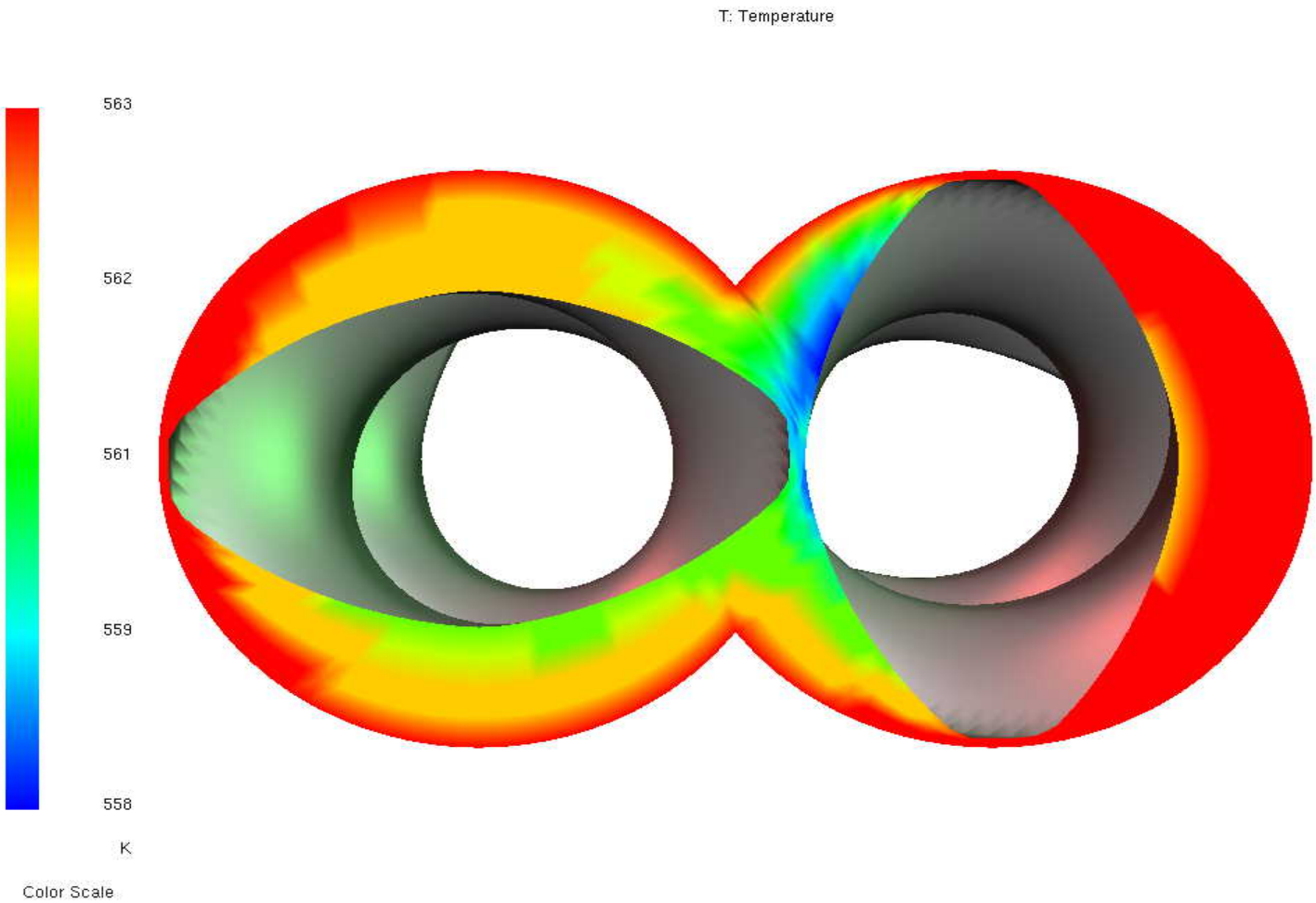

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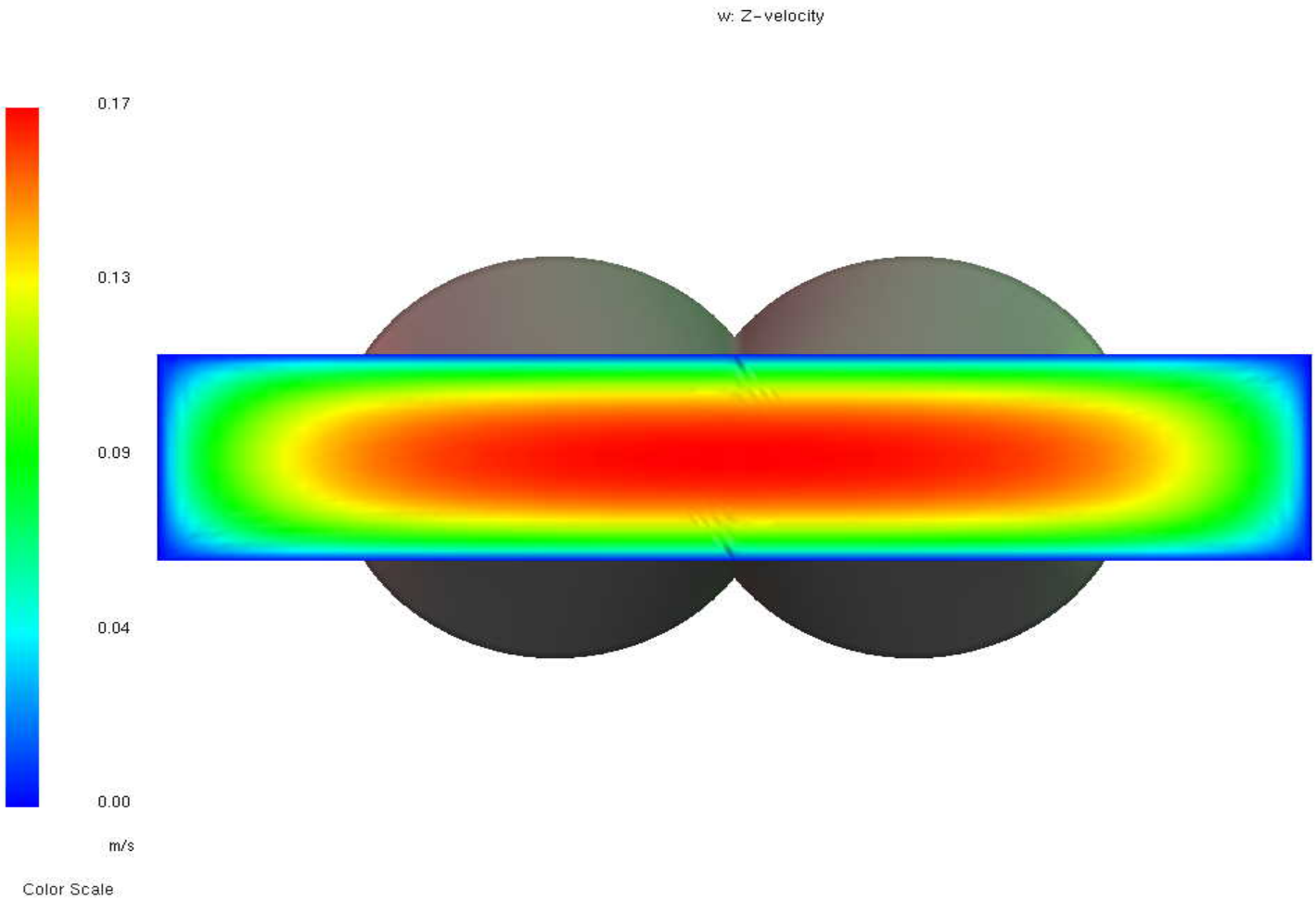

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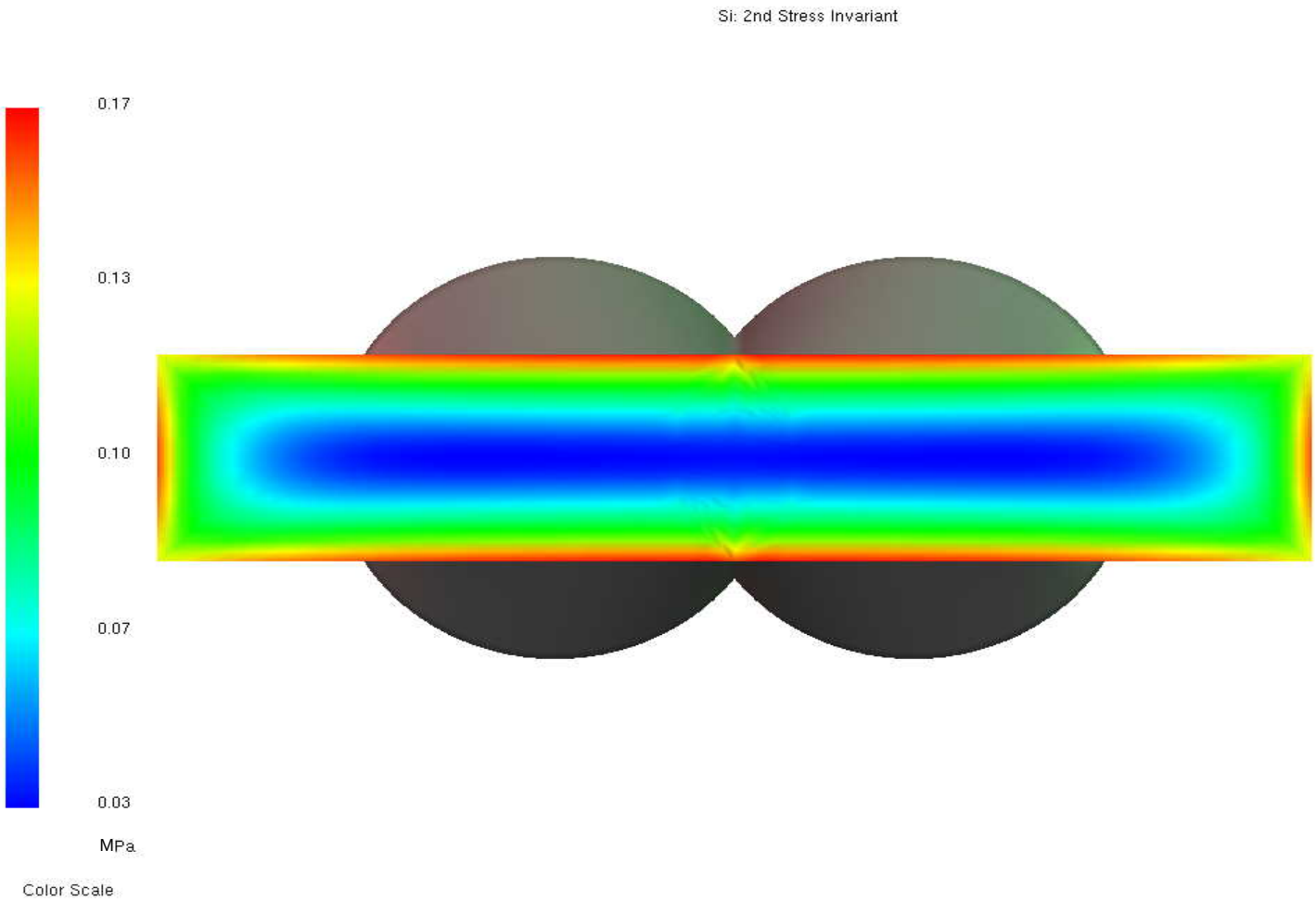

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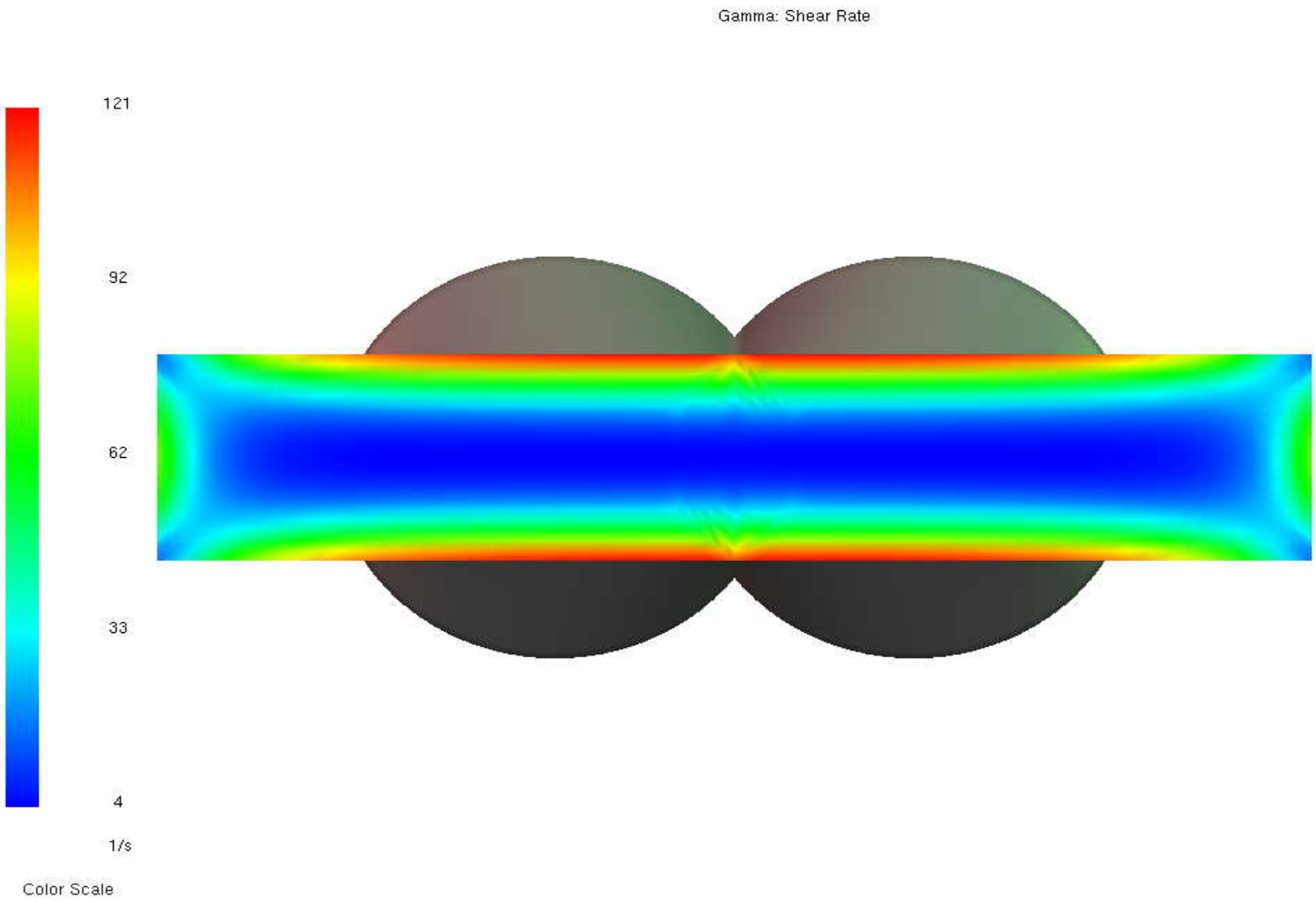

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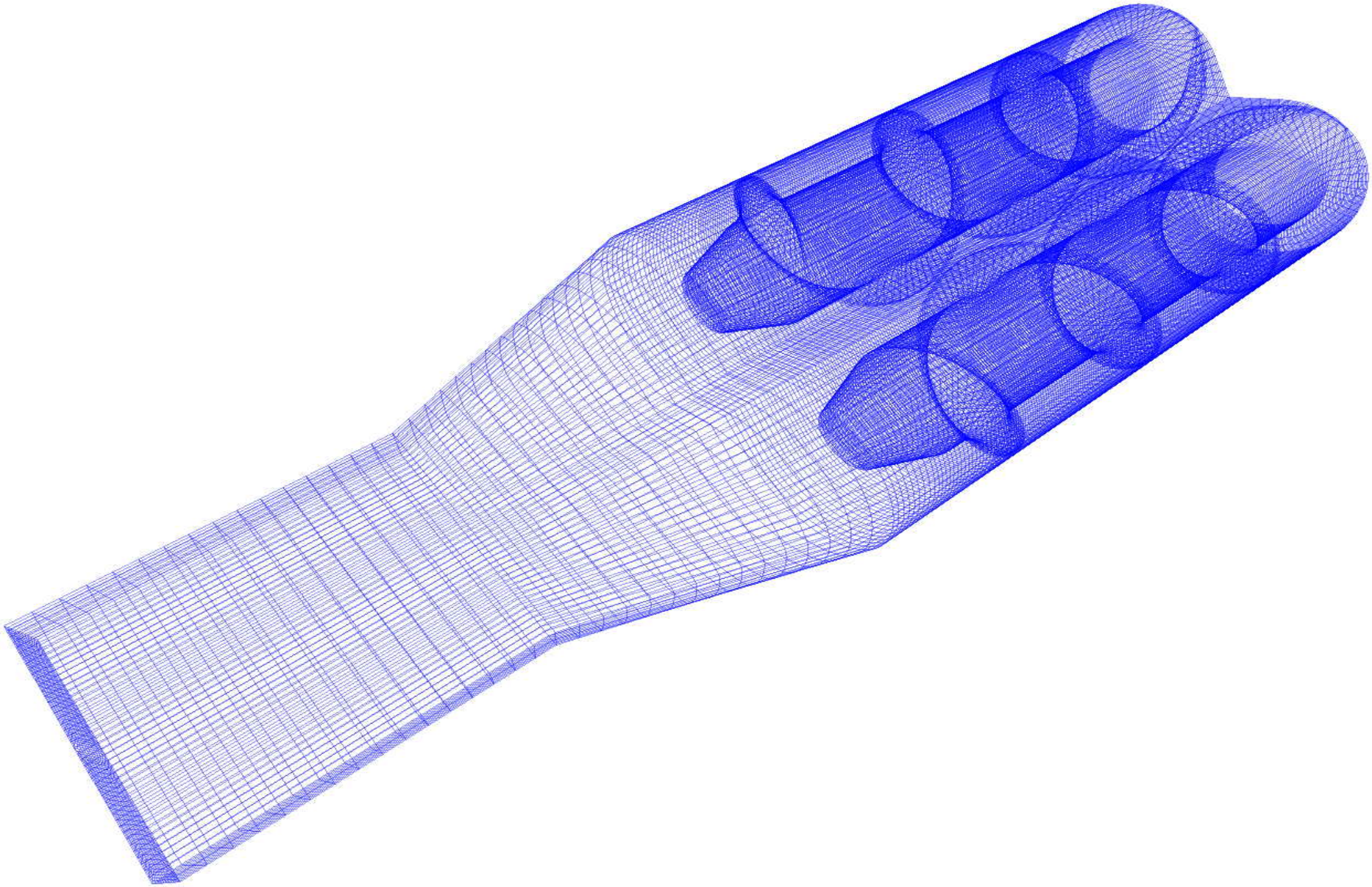
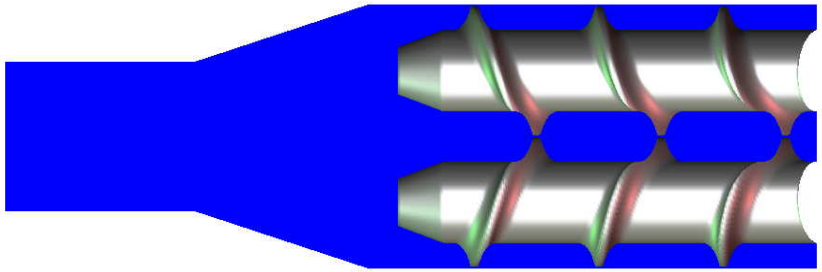
Counter-rotating Tangential Twin Screw Extruder Non-Isothermal FEM Simulation

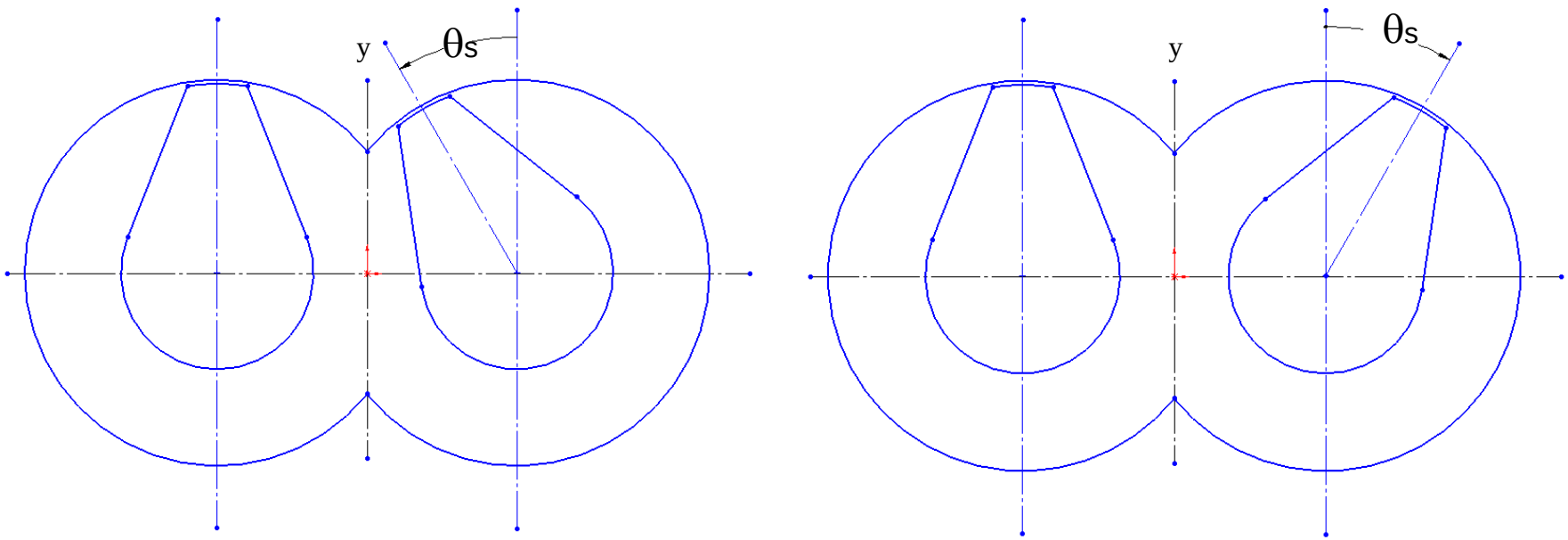


FEM Mesh



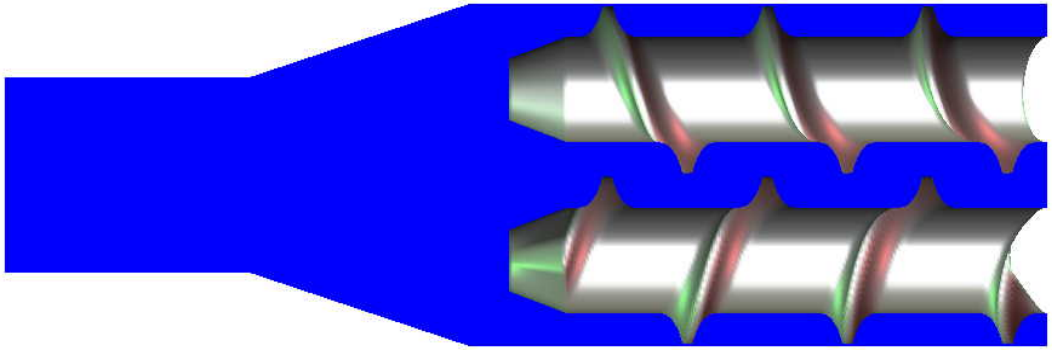
0 degree stagger angle in between the two screws

Counter-rotating, tangential, twin-screw extruder with slit die: Case of matched flights



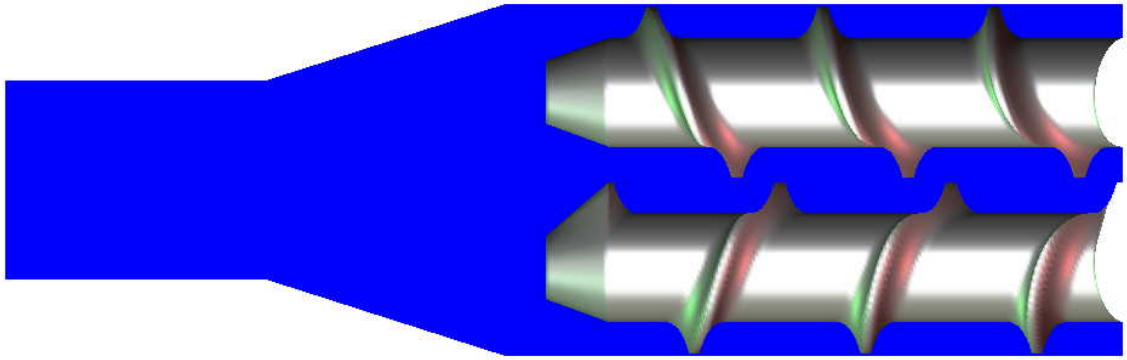
θ_S = Stagger angle

Stagger angle in a counter-rotating, tangential, twin-screw extruder

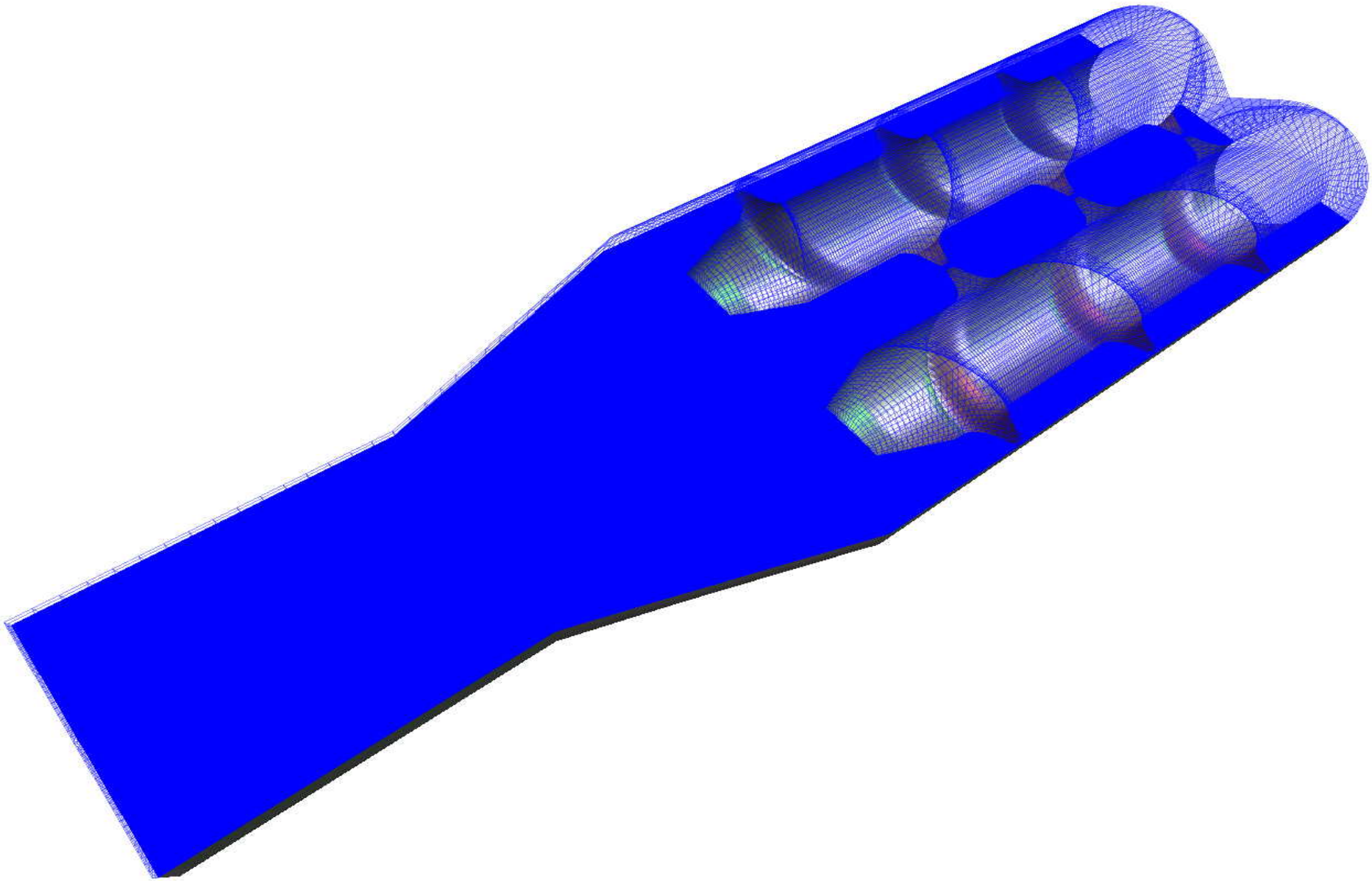


180 degree stagger angle in between the two screws (fully-staggered)

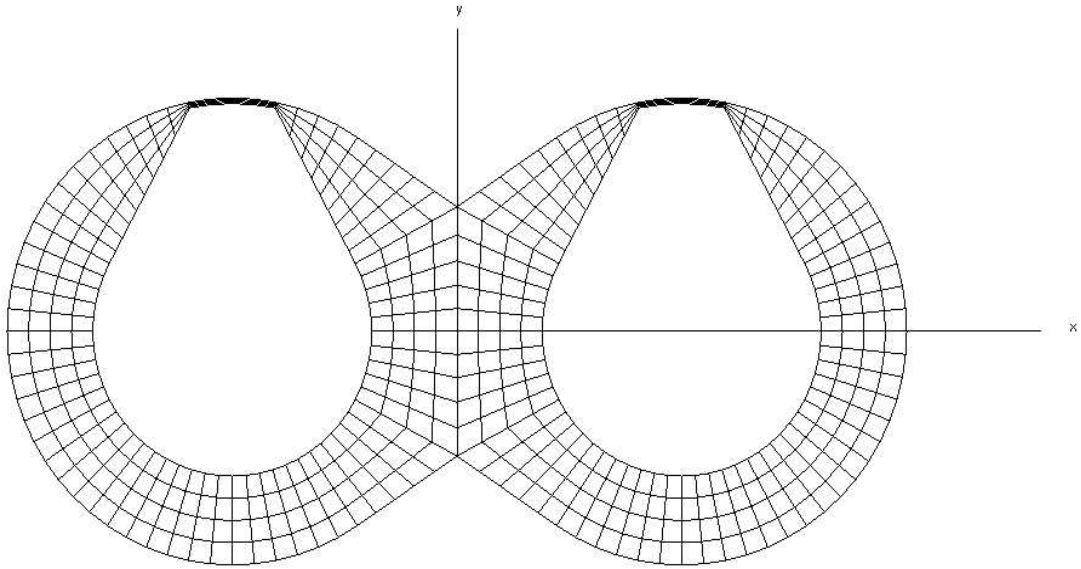
Counter-rotating, tangential, twin-screw extruder with slit die: Case of staggered flights



Counter-rotating, tangential, twin-screw extruder with slit die
Partially staggered flights: Stagger angle = 90 deg

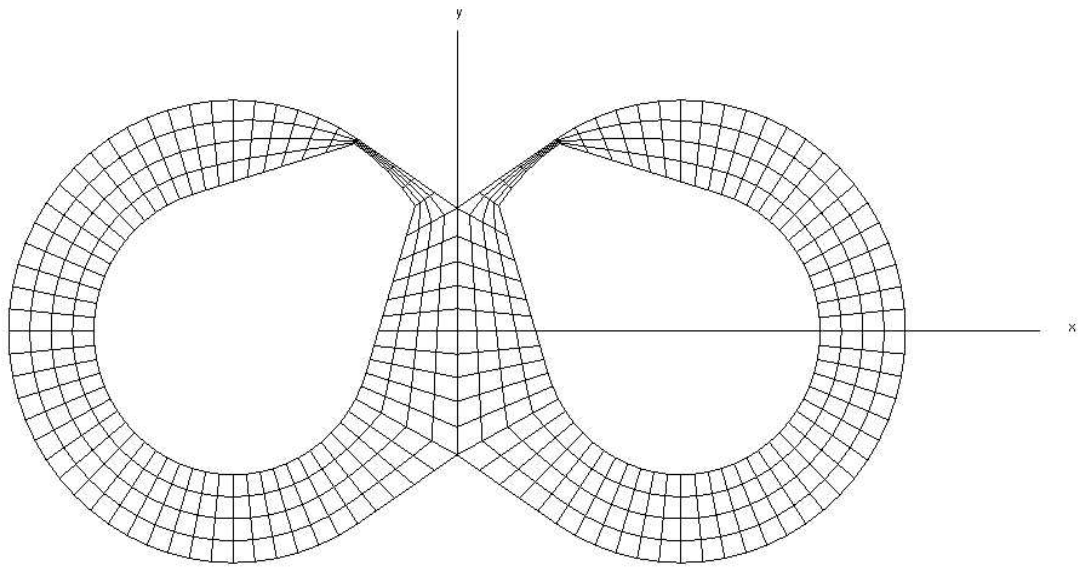


Flow Channel Cutaway

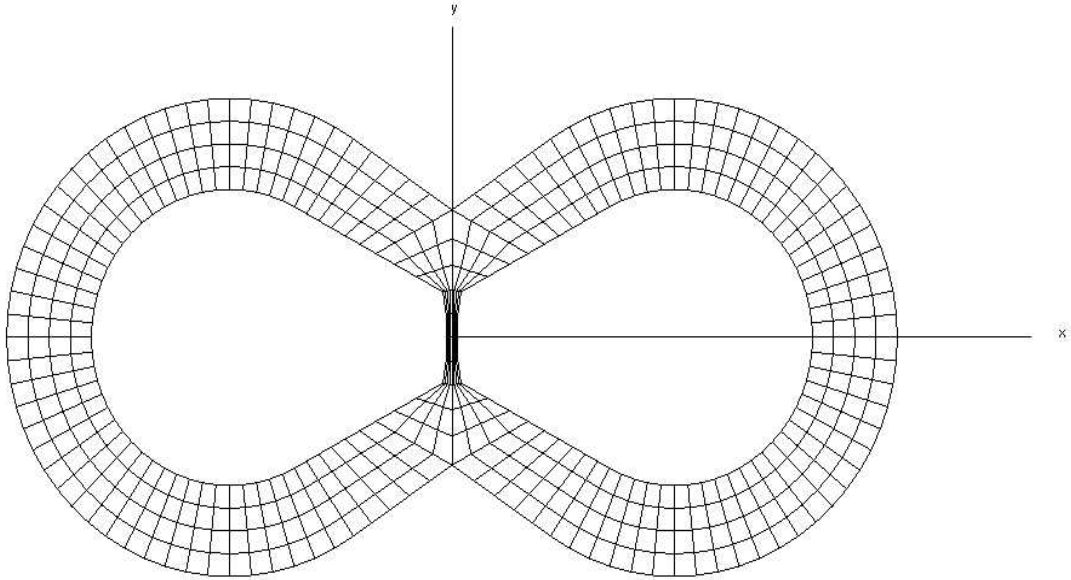


Mesh development for the zero degree stagger

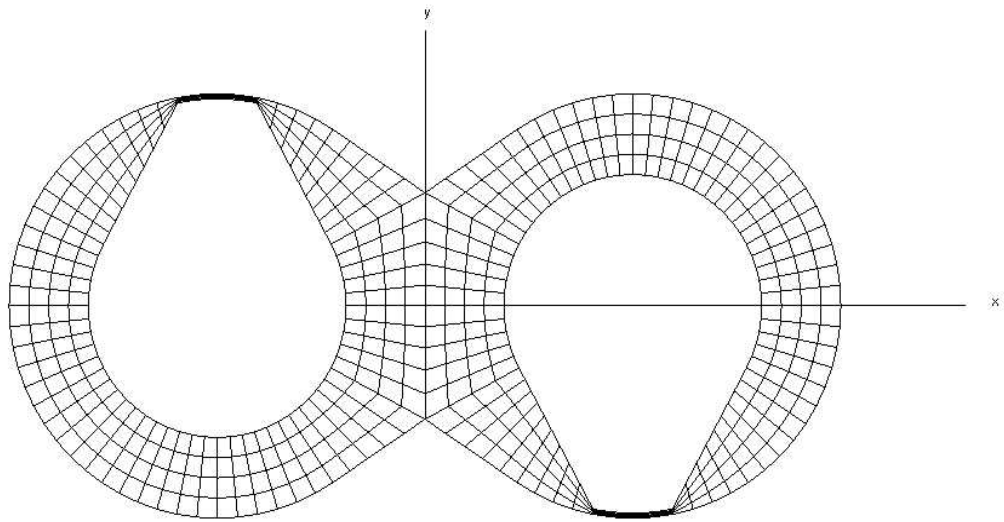
Cross-sectional mesh of twin screws with matched flights at z = 0



Cross-sectional mesh of twin screws with matched flights at z = L/8

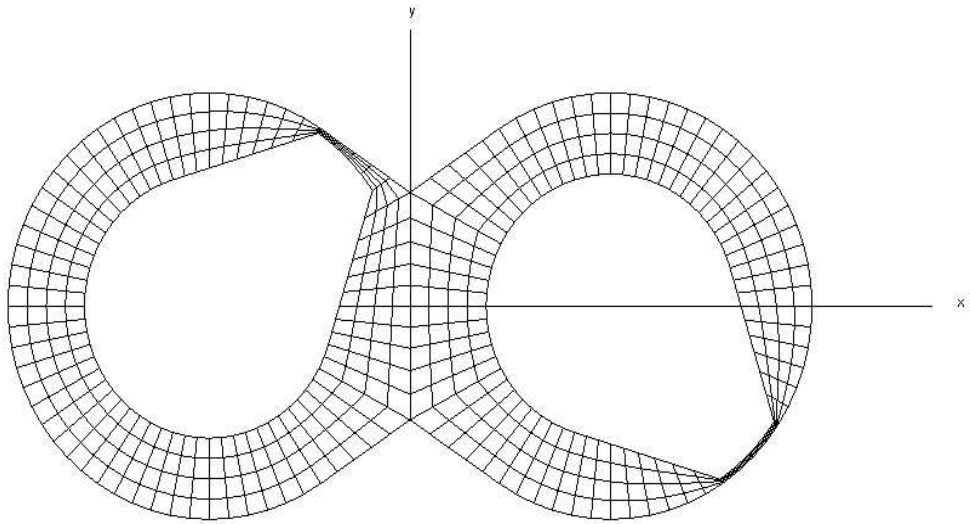


Cross-sectional mesh of twin screws with matched flights at z = Lead/4,

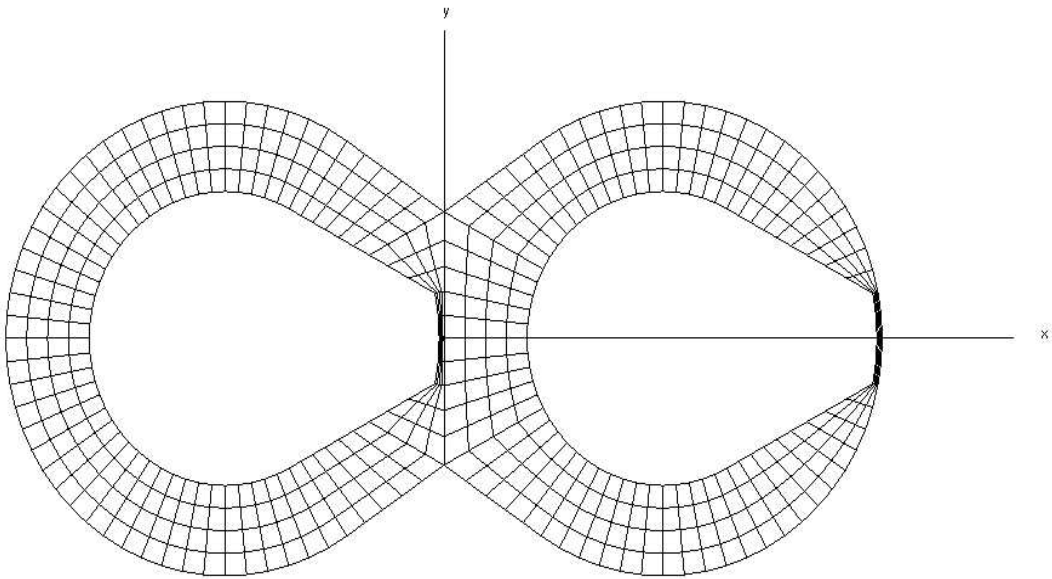


Mesh development for 180 stagger

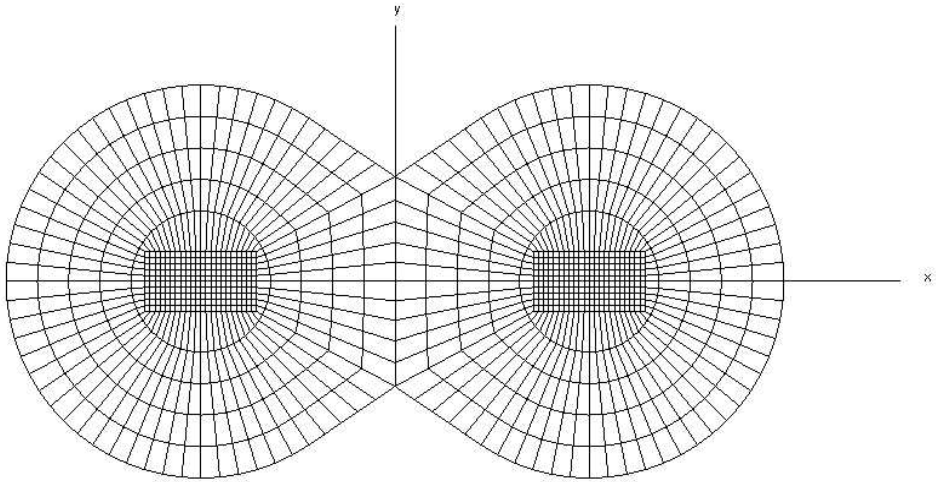
Cross-sectional mesh of twin screws with fully-staggered flights at z = 0



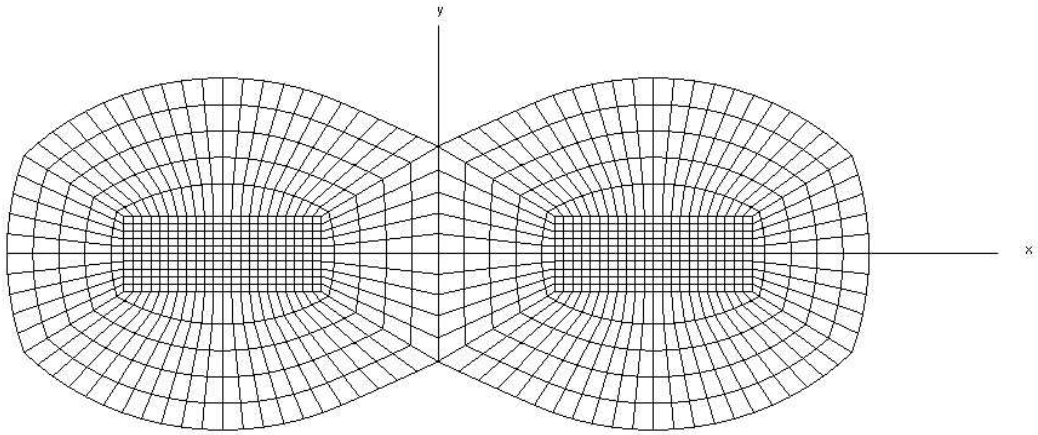
Cross-sectional mesh of twin screws with fully-staggered flights at z = L/8



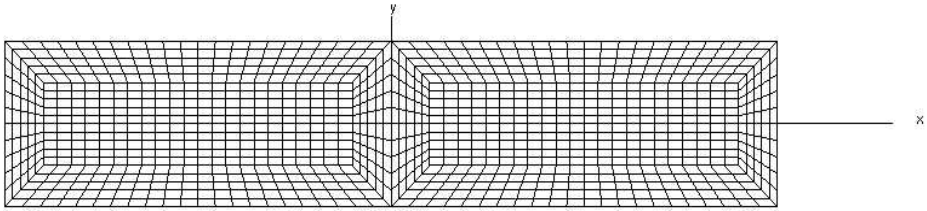
Cross-sectional mesh of twin screws with fully-staggered flights at z = L/4



Cross-sectional mesh at the entrance of converging section of the die



Cross-sectional mesh at the middle of converging section of the die



Cross-sectional mesh in the slit of the die

Terminology/Notation

dof = Degree of fill; Number of leads full

L = Screw lead

m_0 = Consistency index, Pa-s^n
= 10,000 Pa-s^n, assumed for present simulations

n = Power law exponent

N = Extruder speed, rpm

p = Pressure; p = p(z)

P = Peak pressure

Q = Flow rate

R = Screw (flight) radius

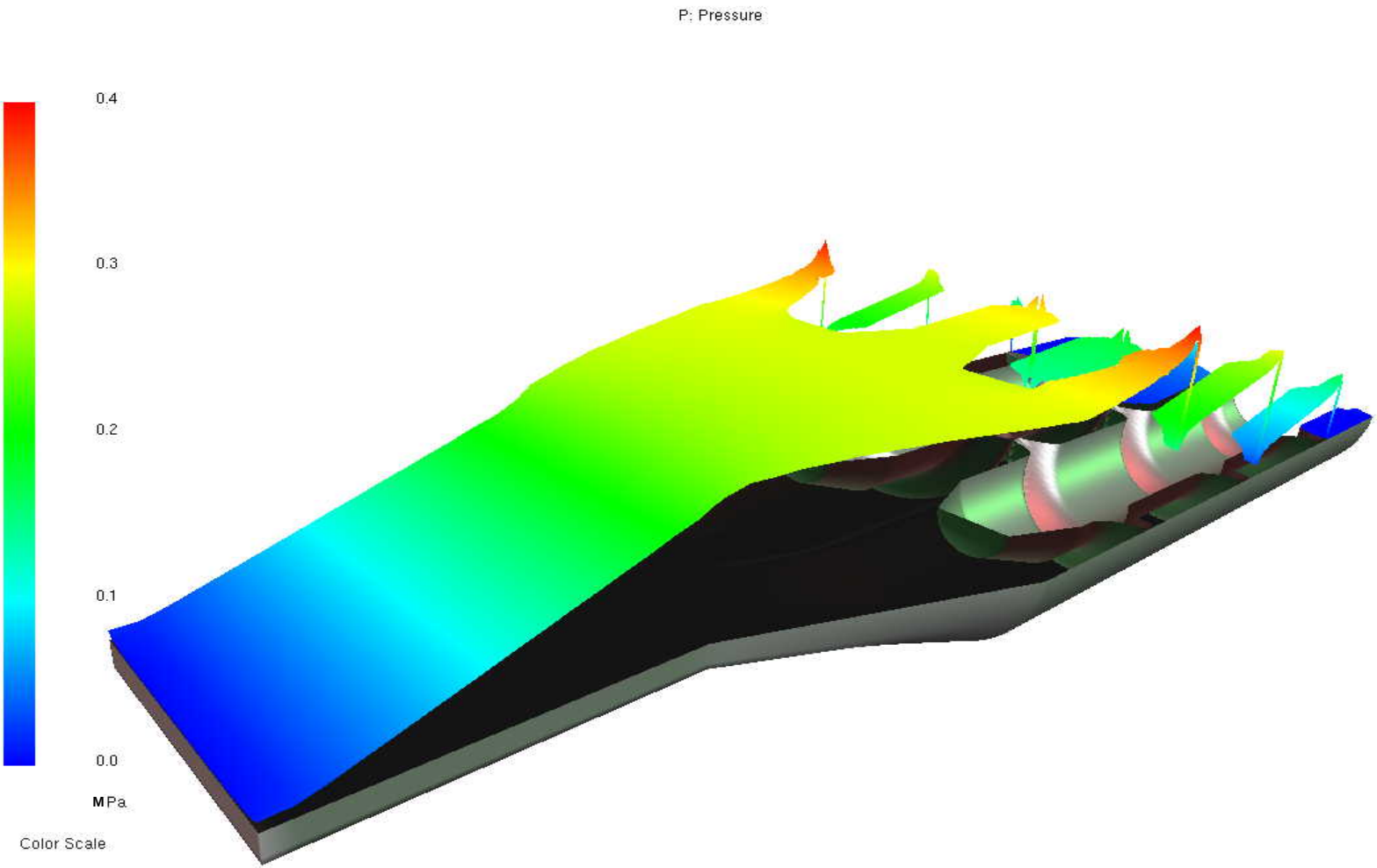
T = Temperature, K

T_{in} = Inlet temperature
= 453 K, assumed for present simulations

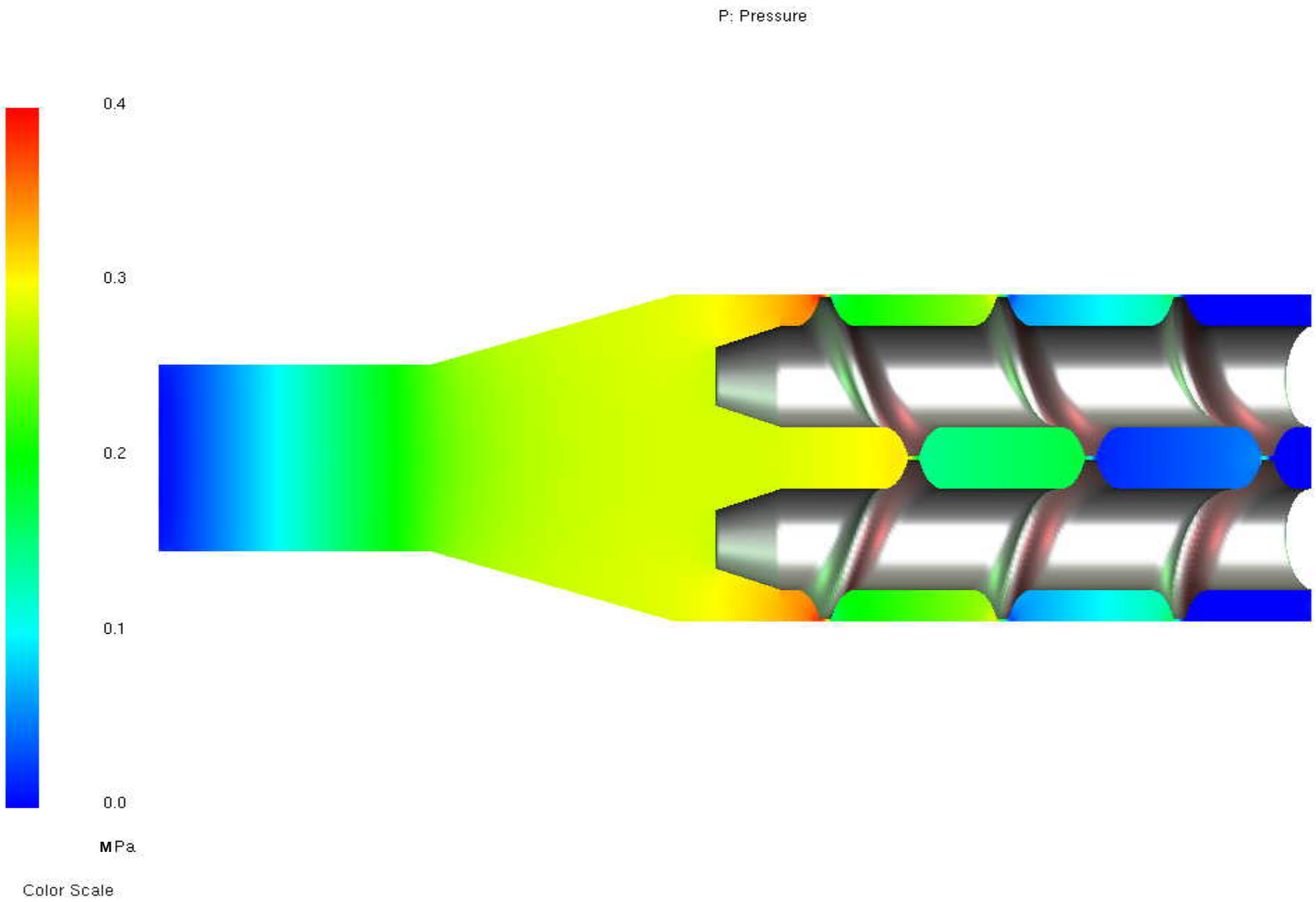
T_{wall} = Inside wall surface temperature of Extruder and die, K

z = Distance along extruder axis

$\omega = 2\pi N/60$; angular speed, rad/s



3 leads, 100 RPM, 123 lb/hr, 180°C, P_{max} = 222 psi, m = 10,000 Pa-s^n, n = 0.5



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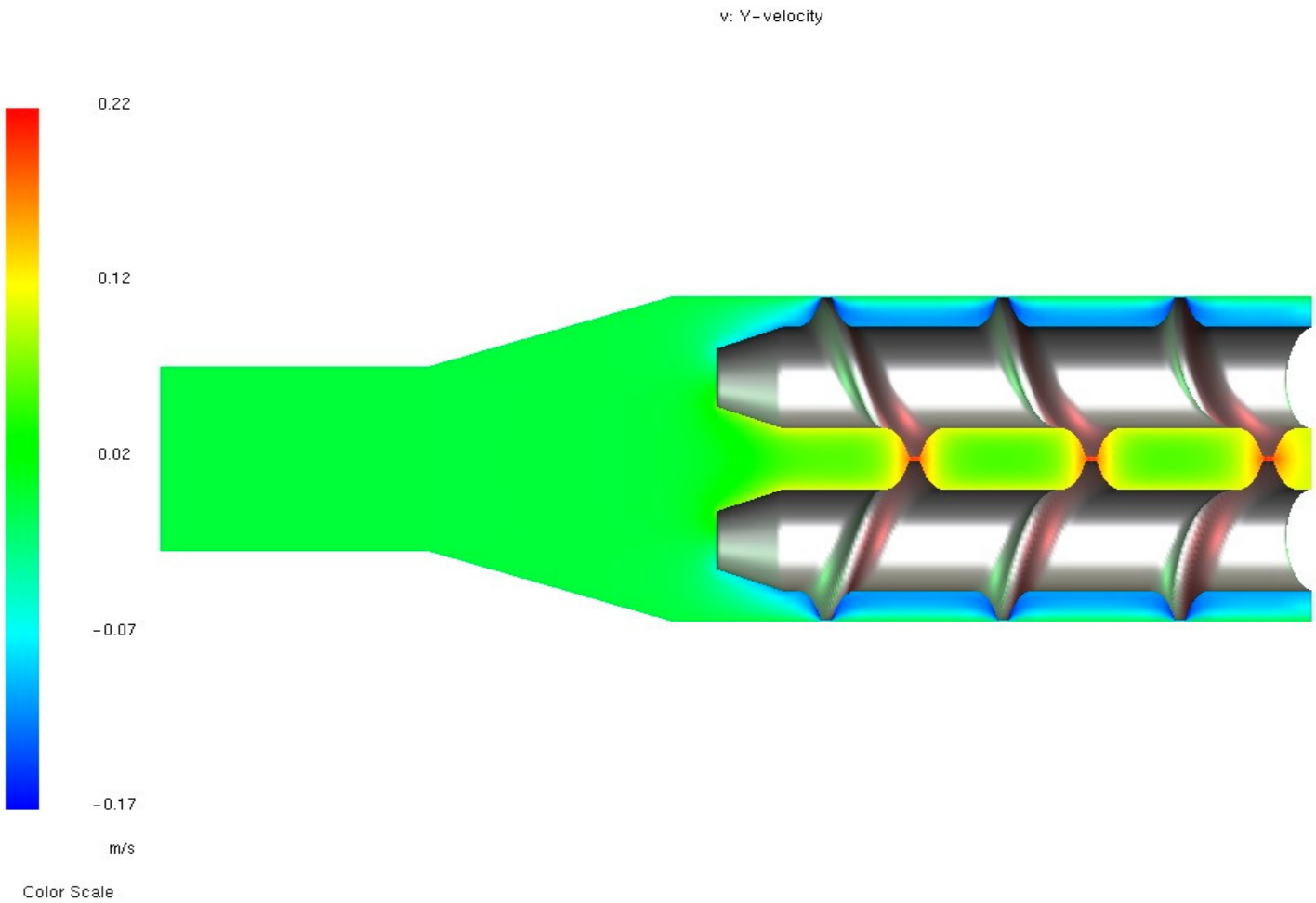

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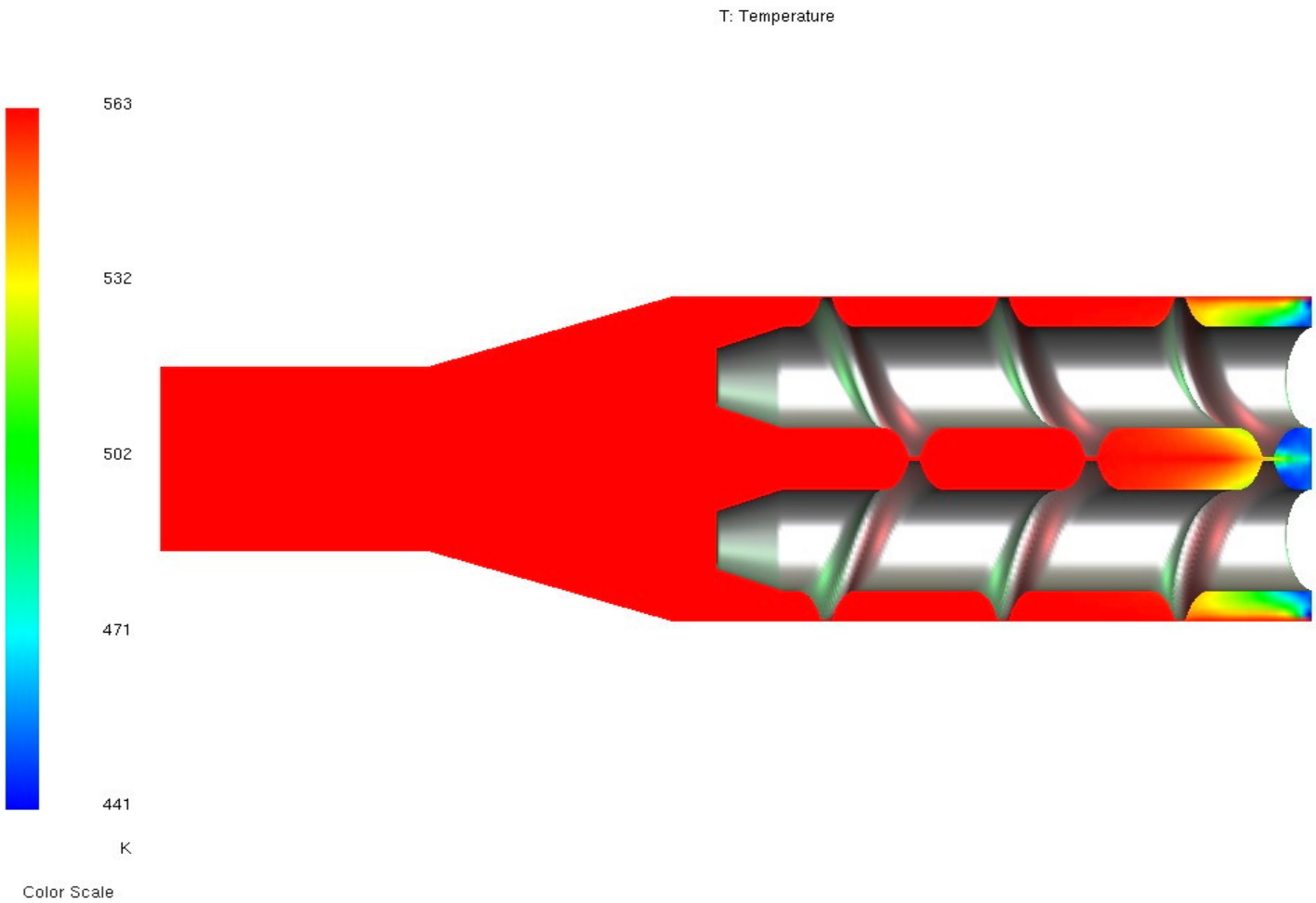

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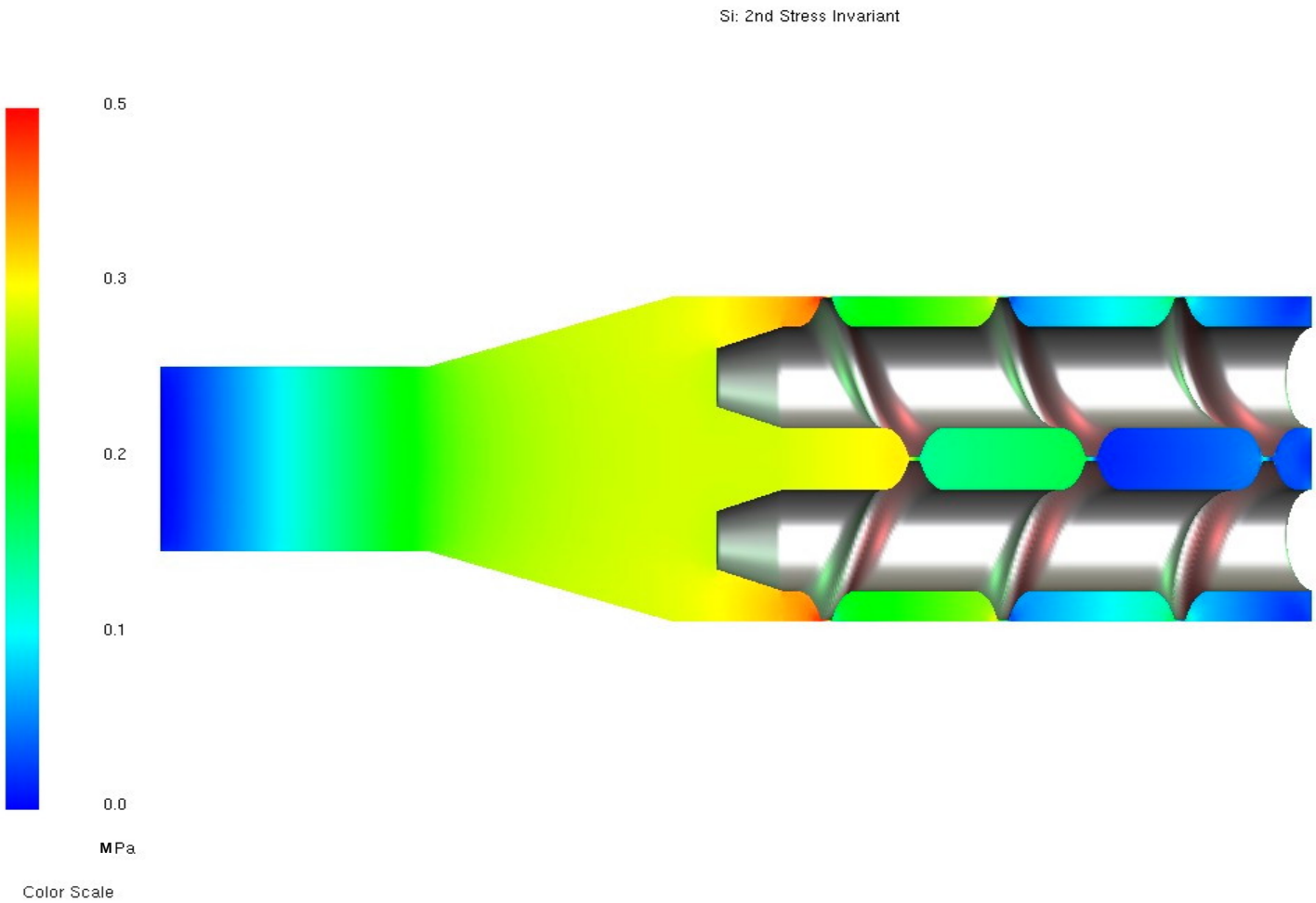

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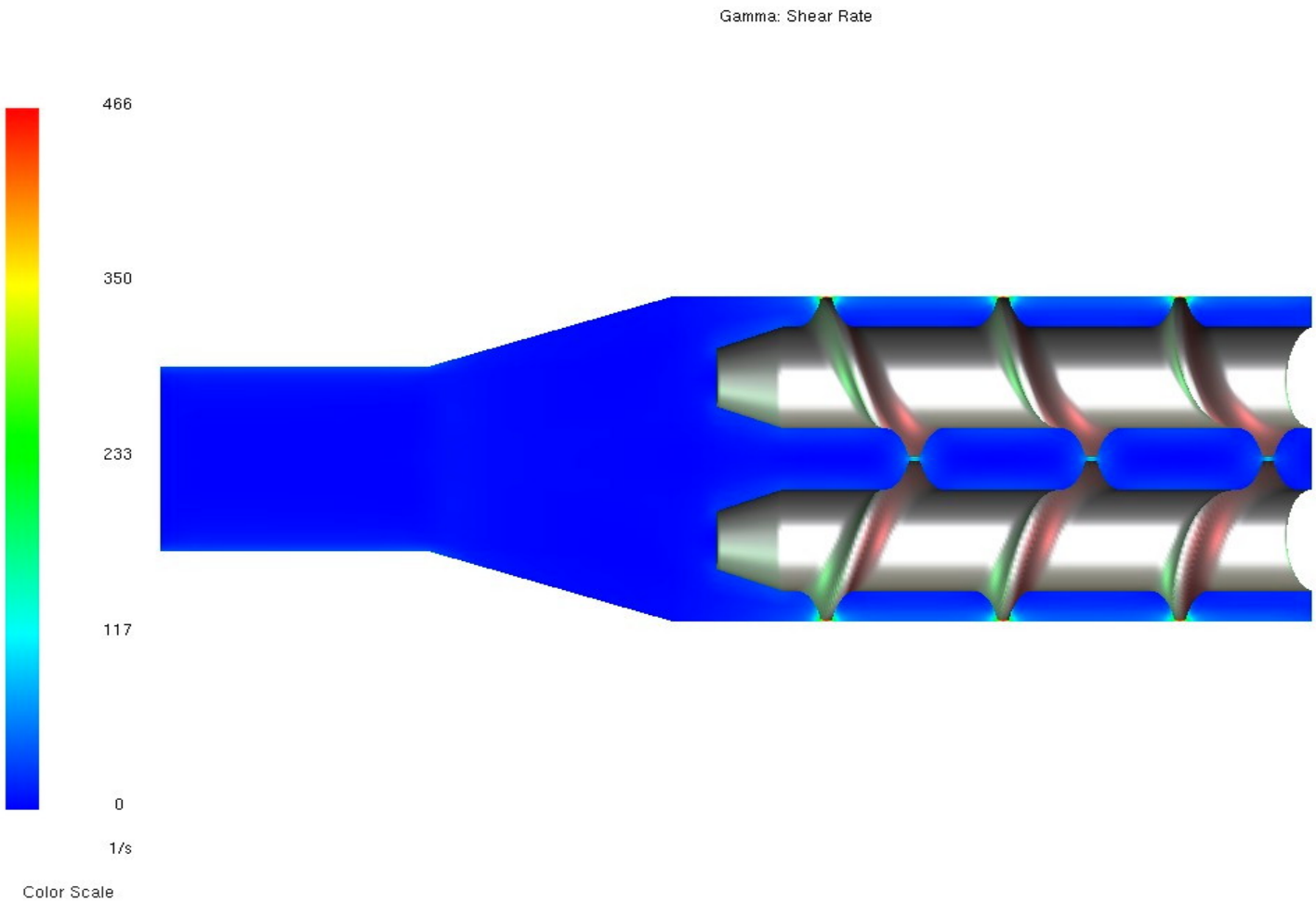

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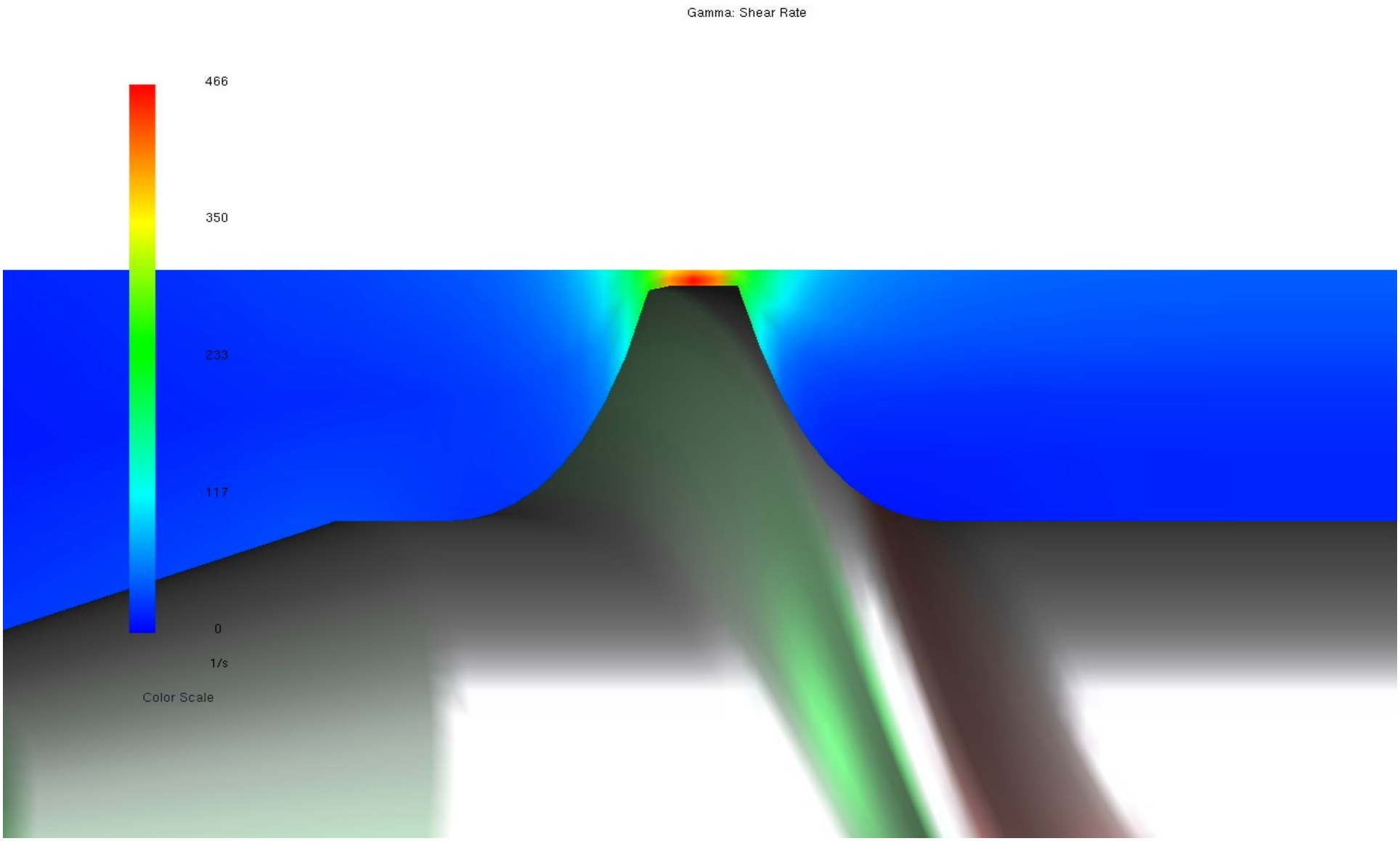

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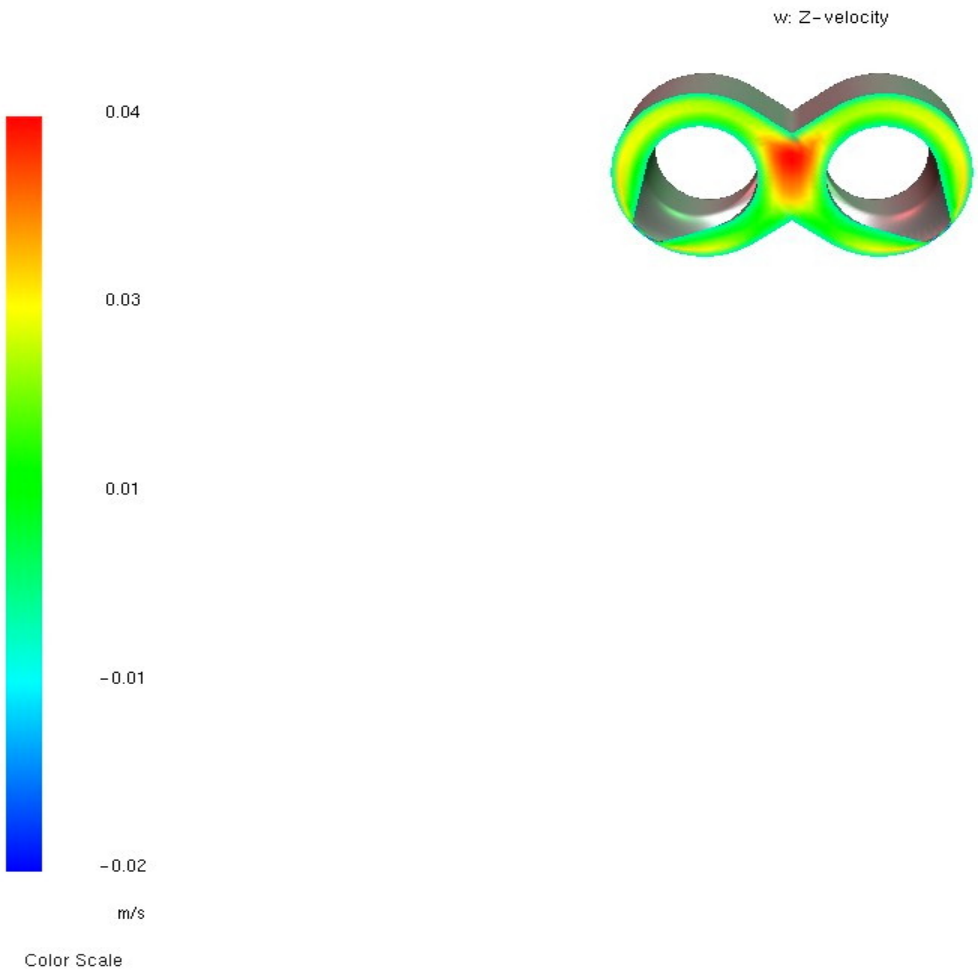

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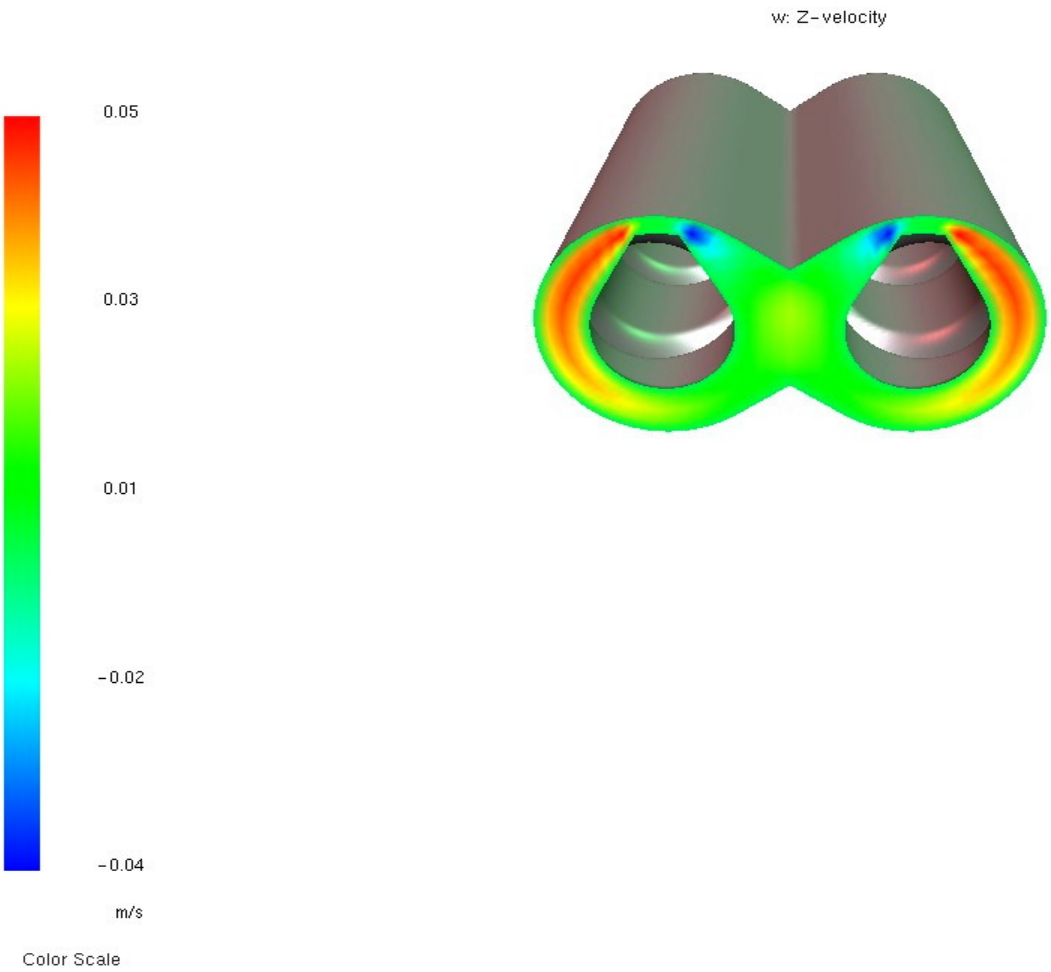

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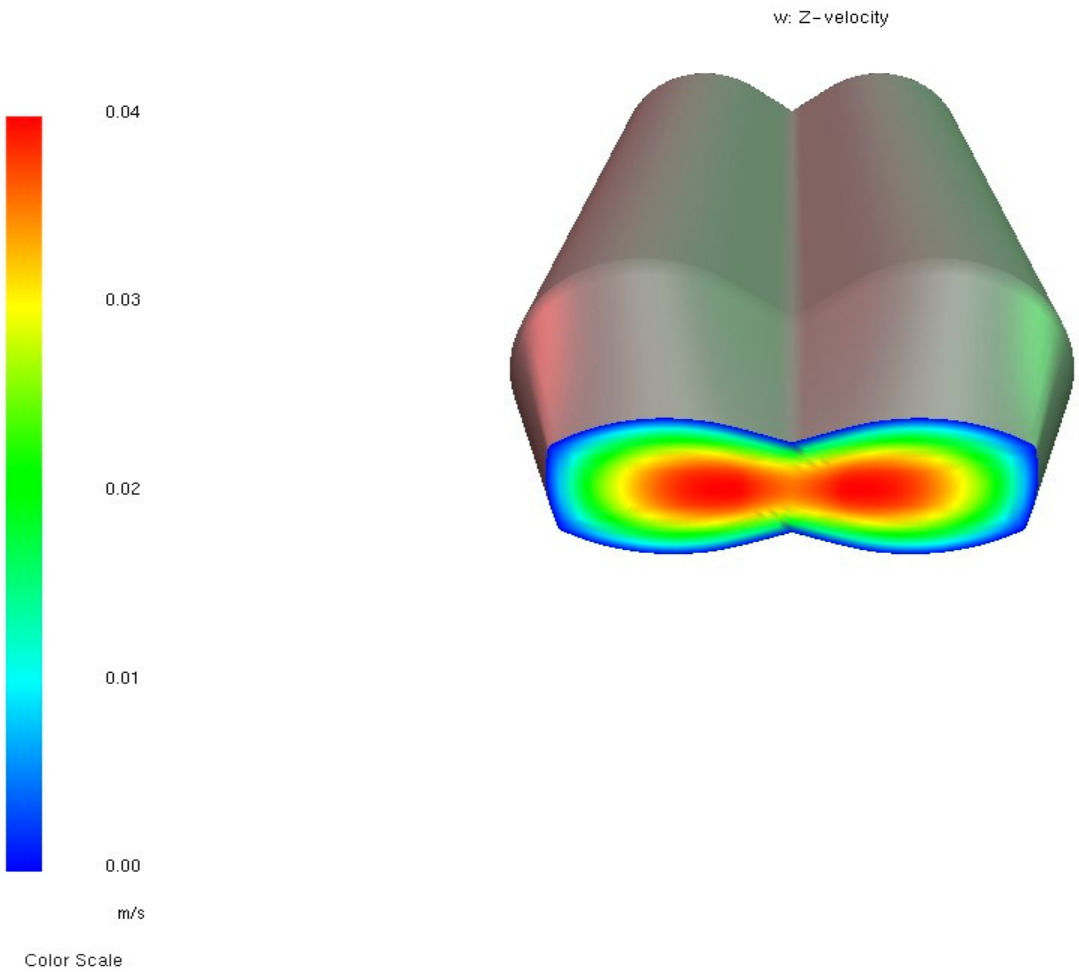

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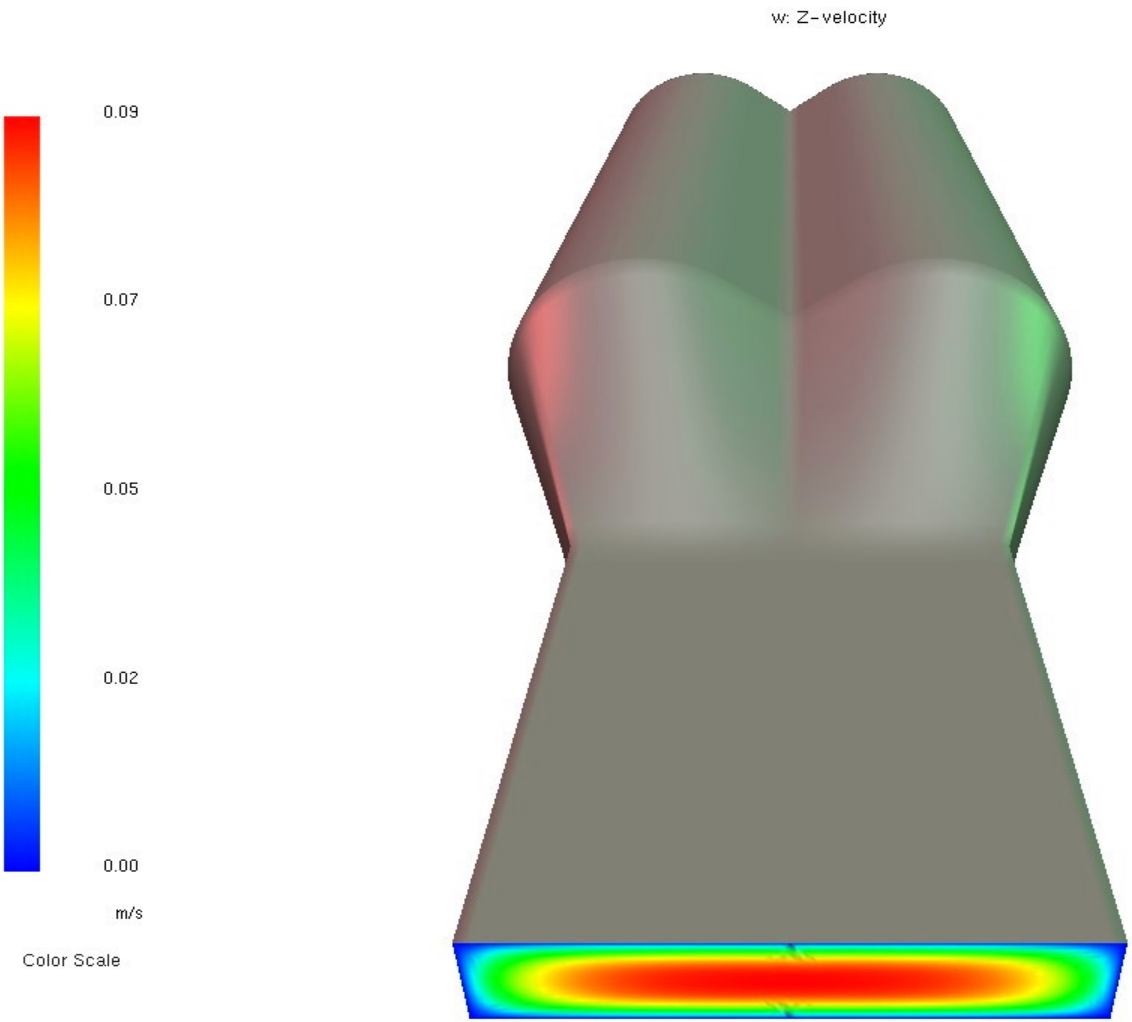

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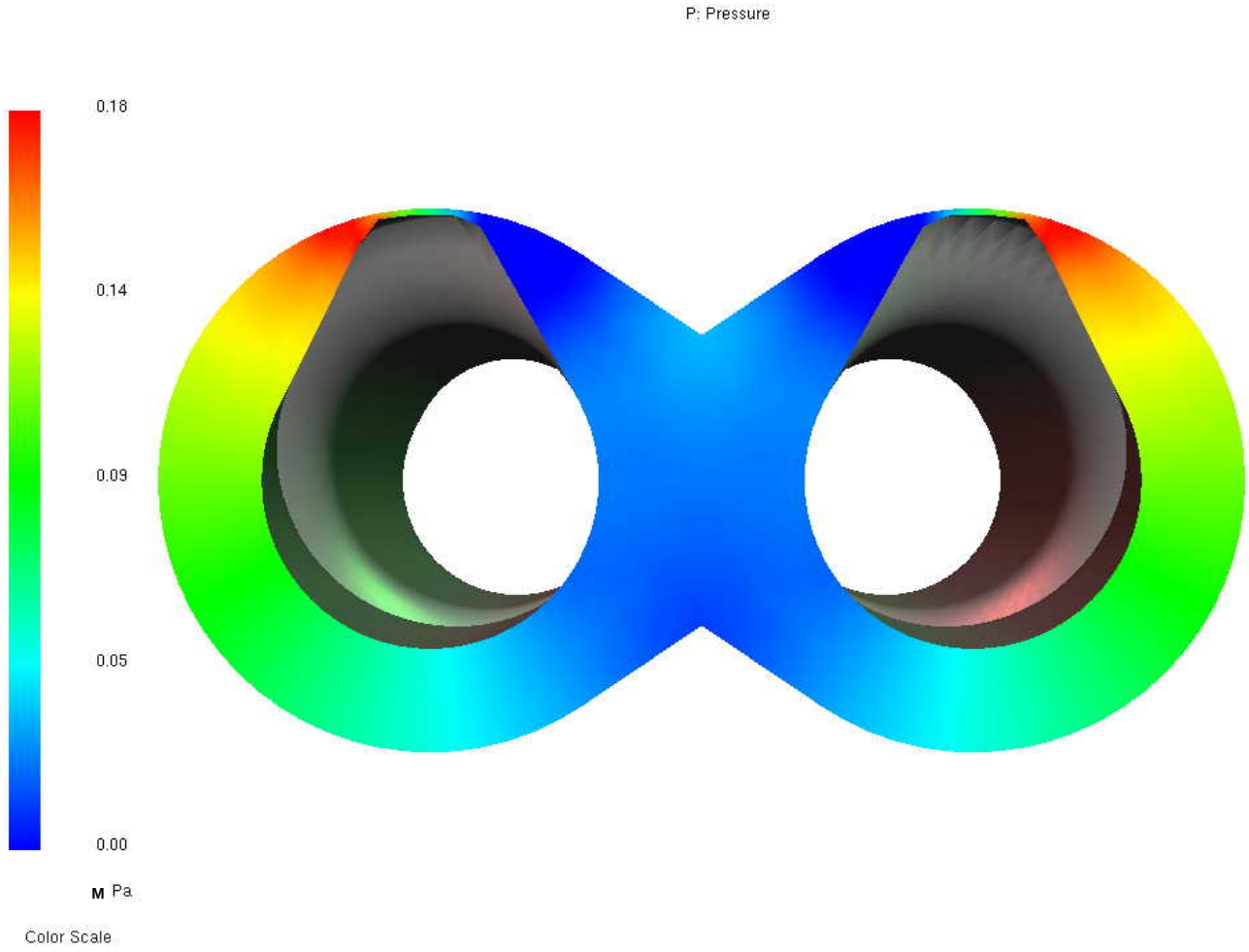

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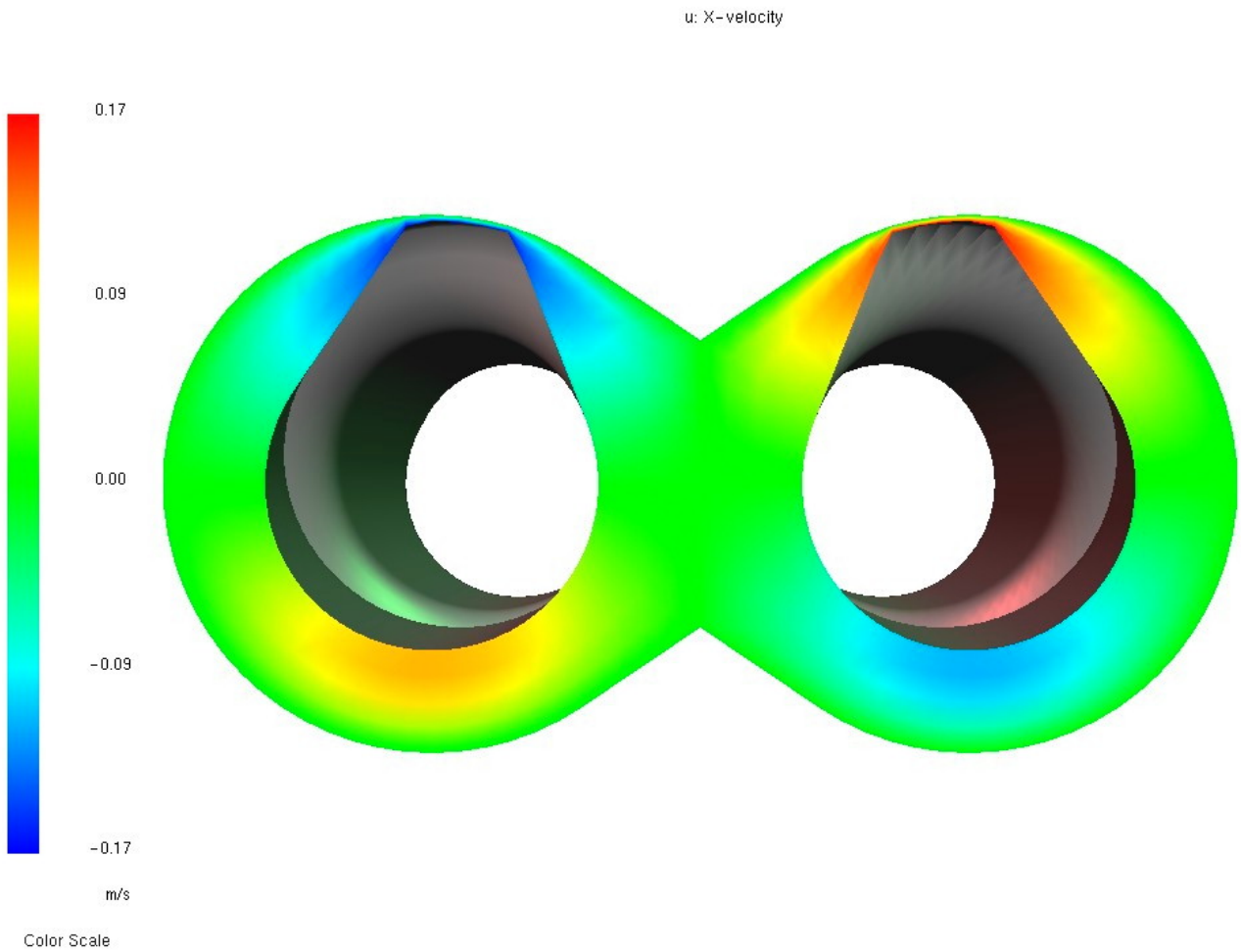

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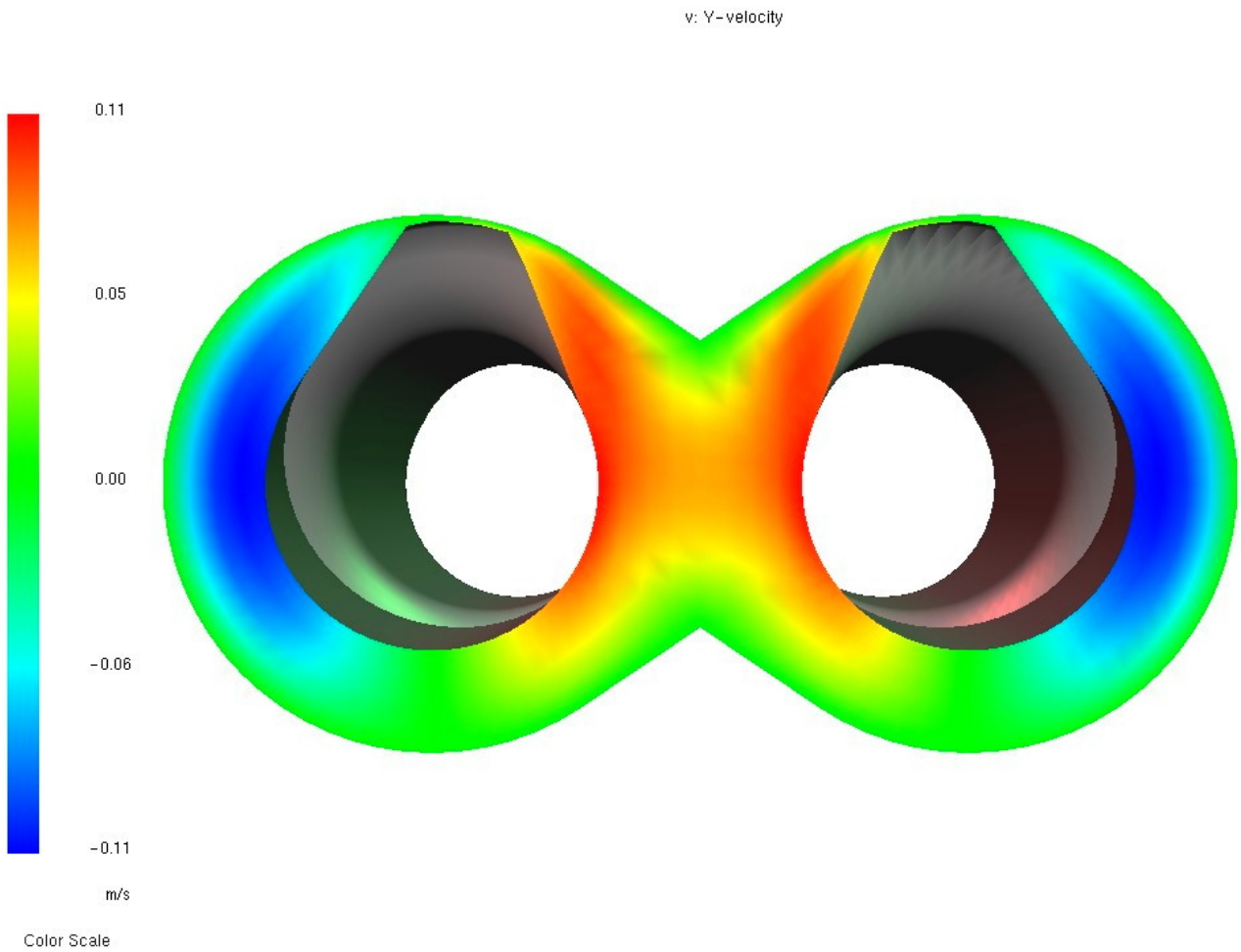

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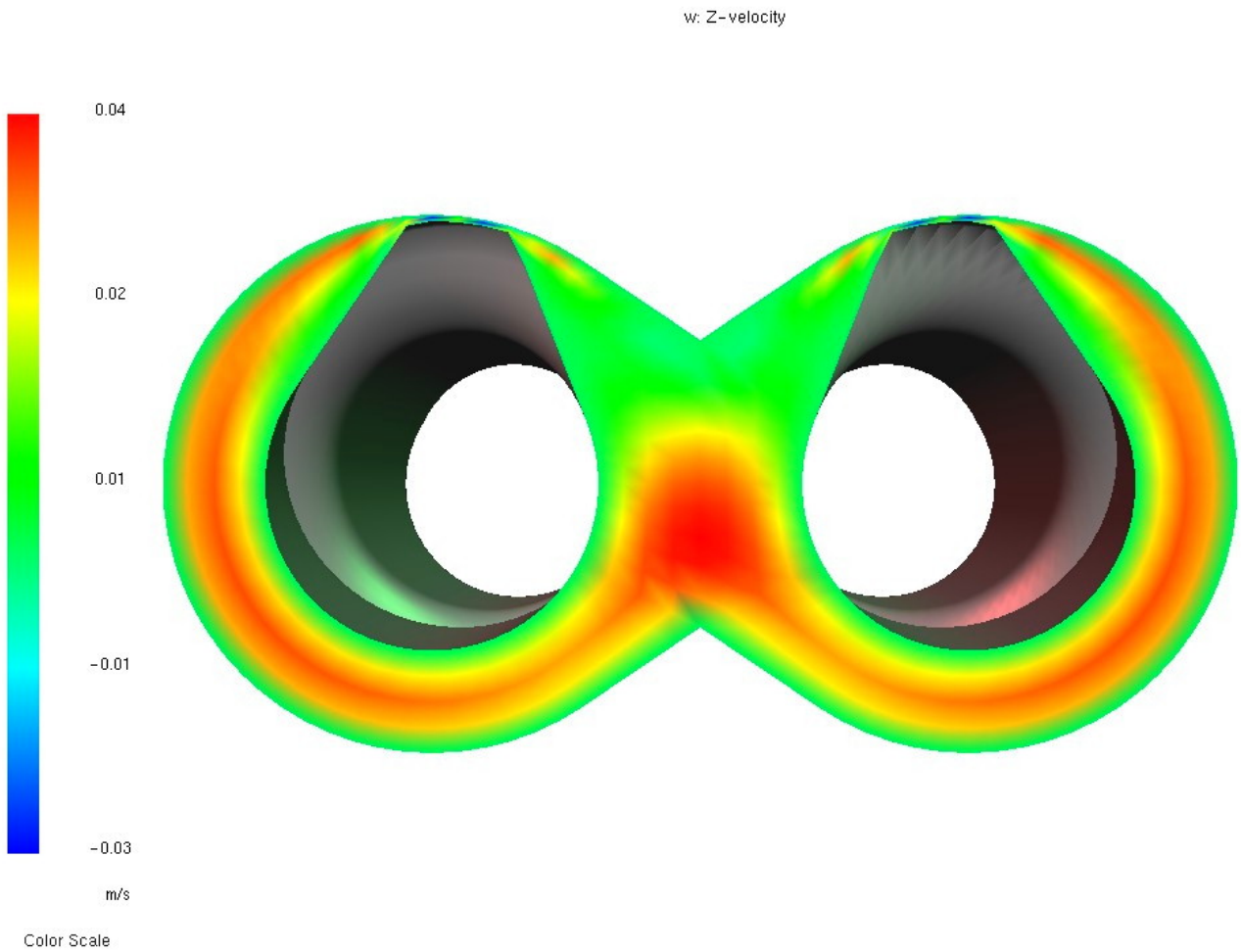

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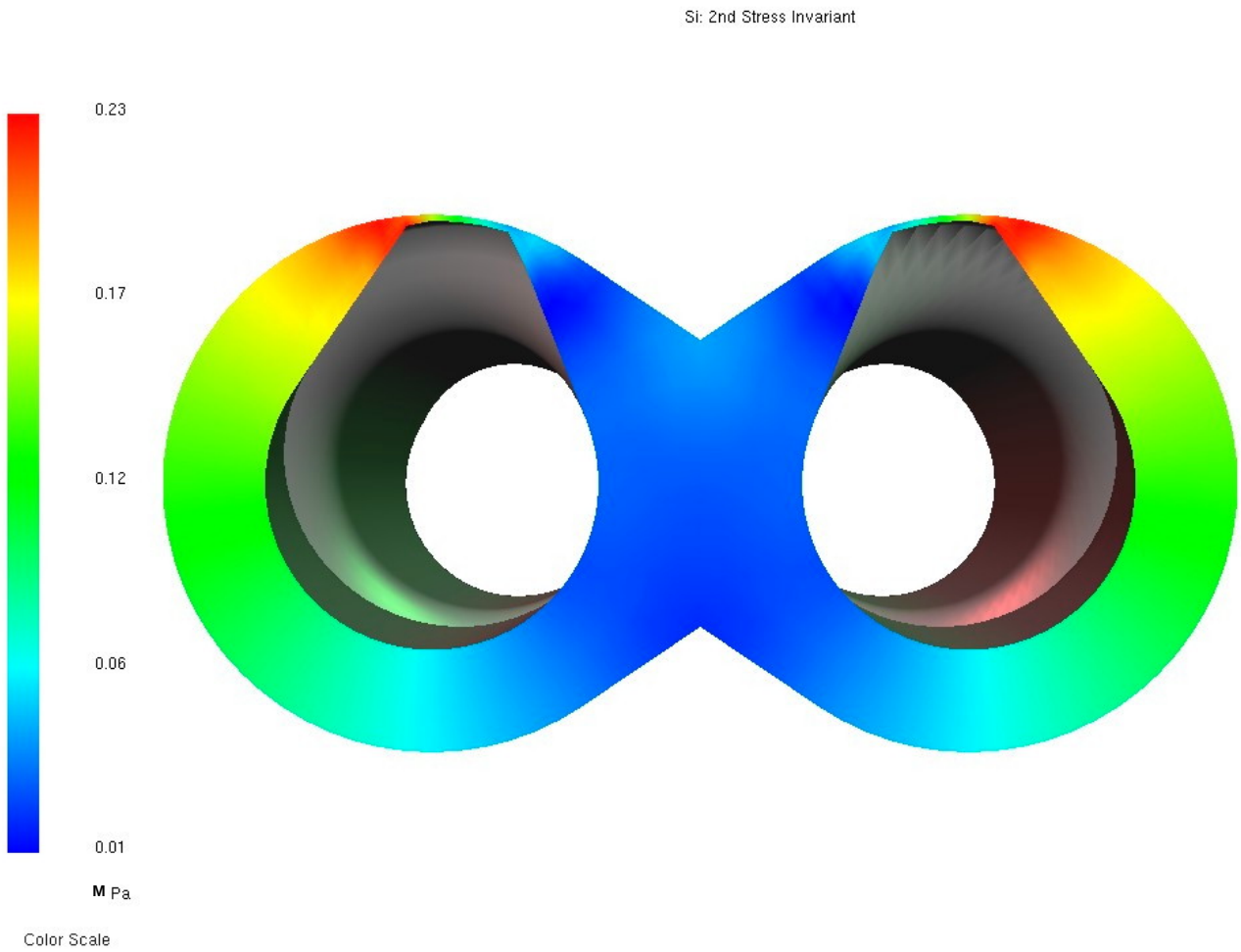

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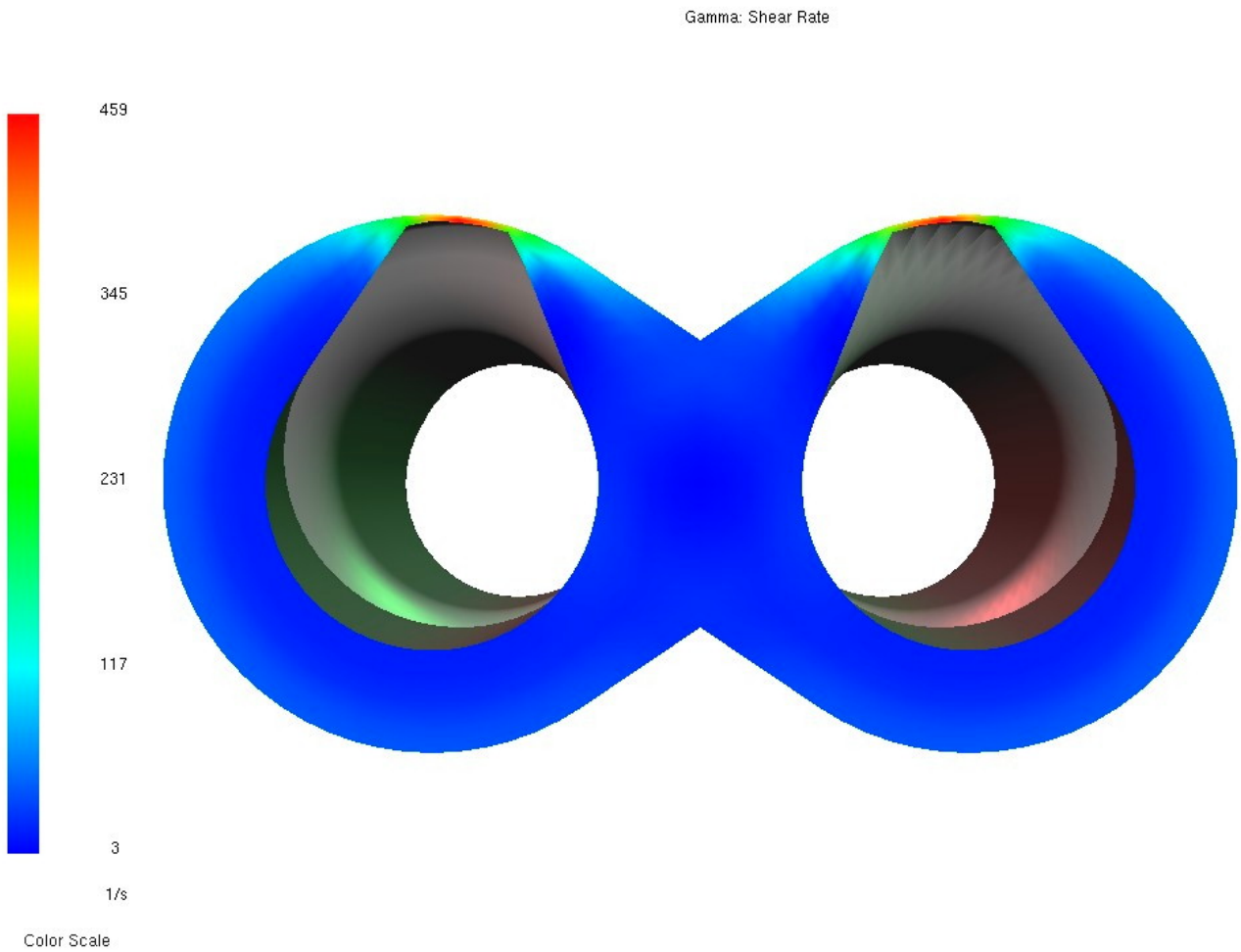

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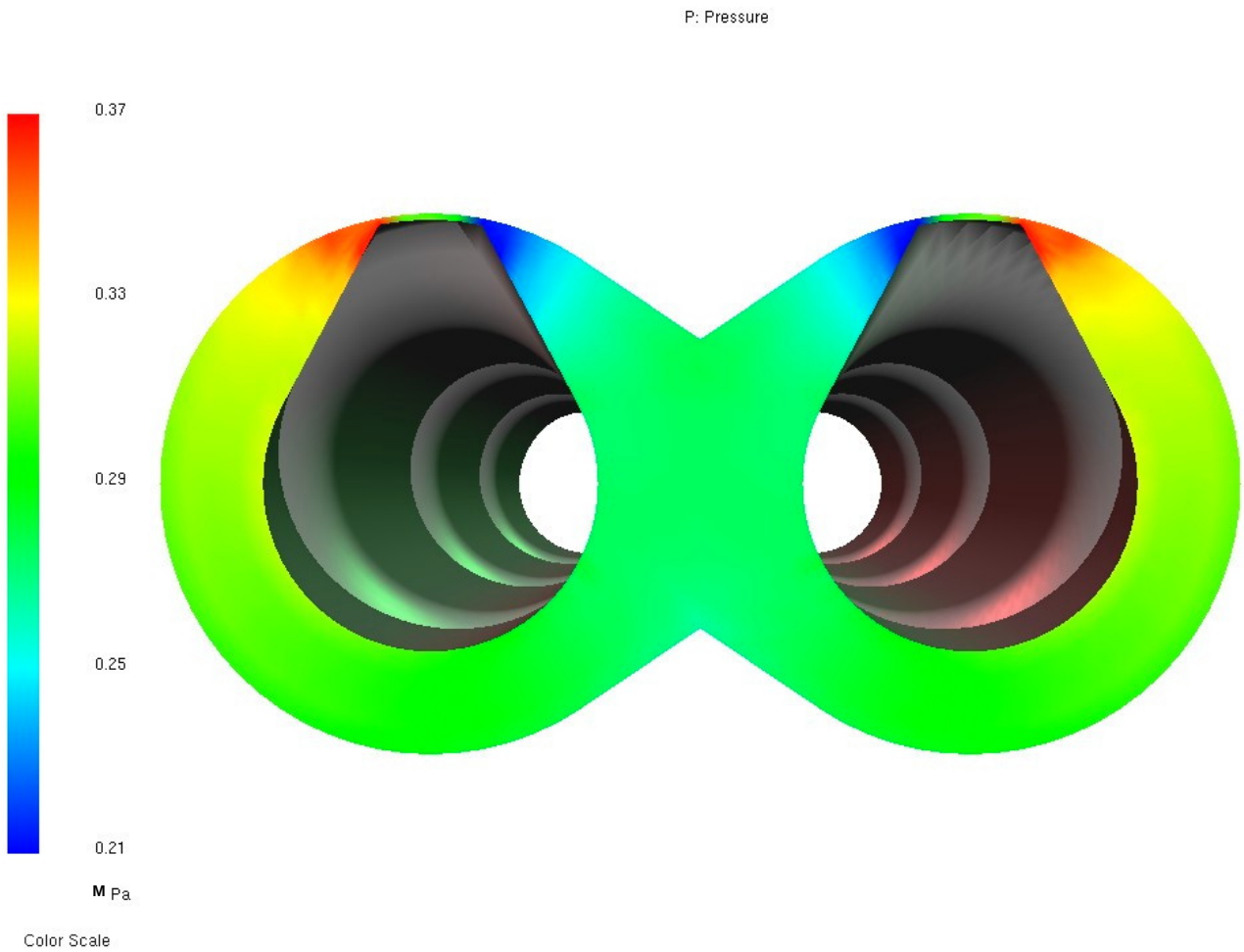

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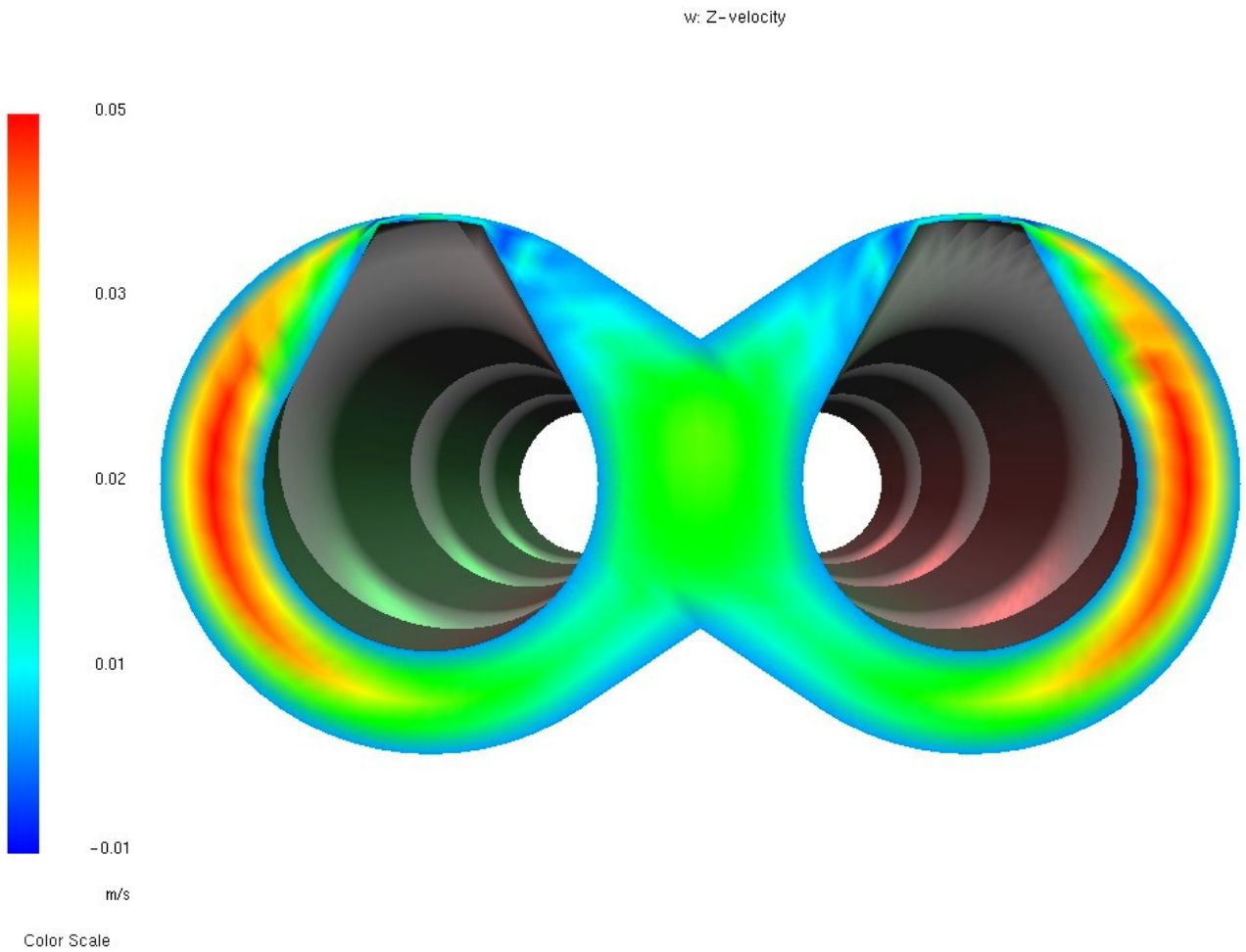

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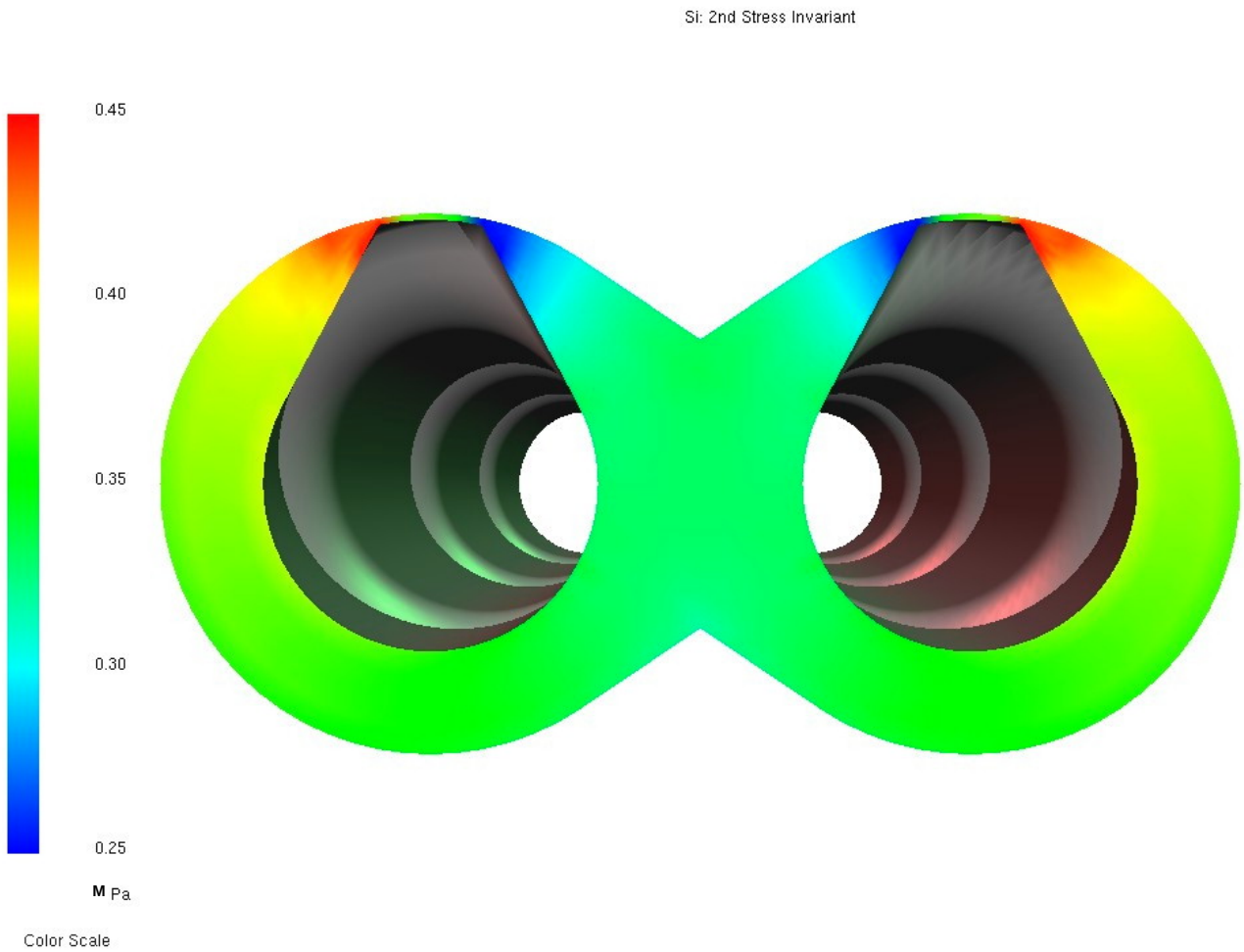

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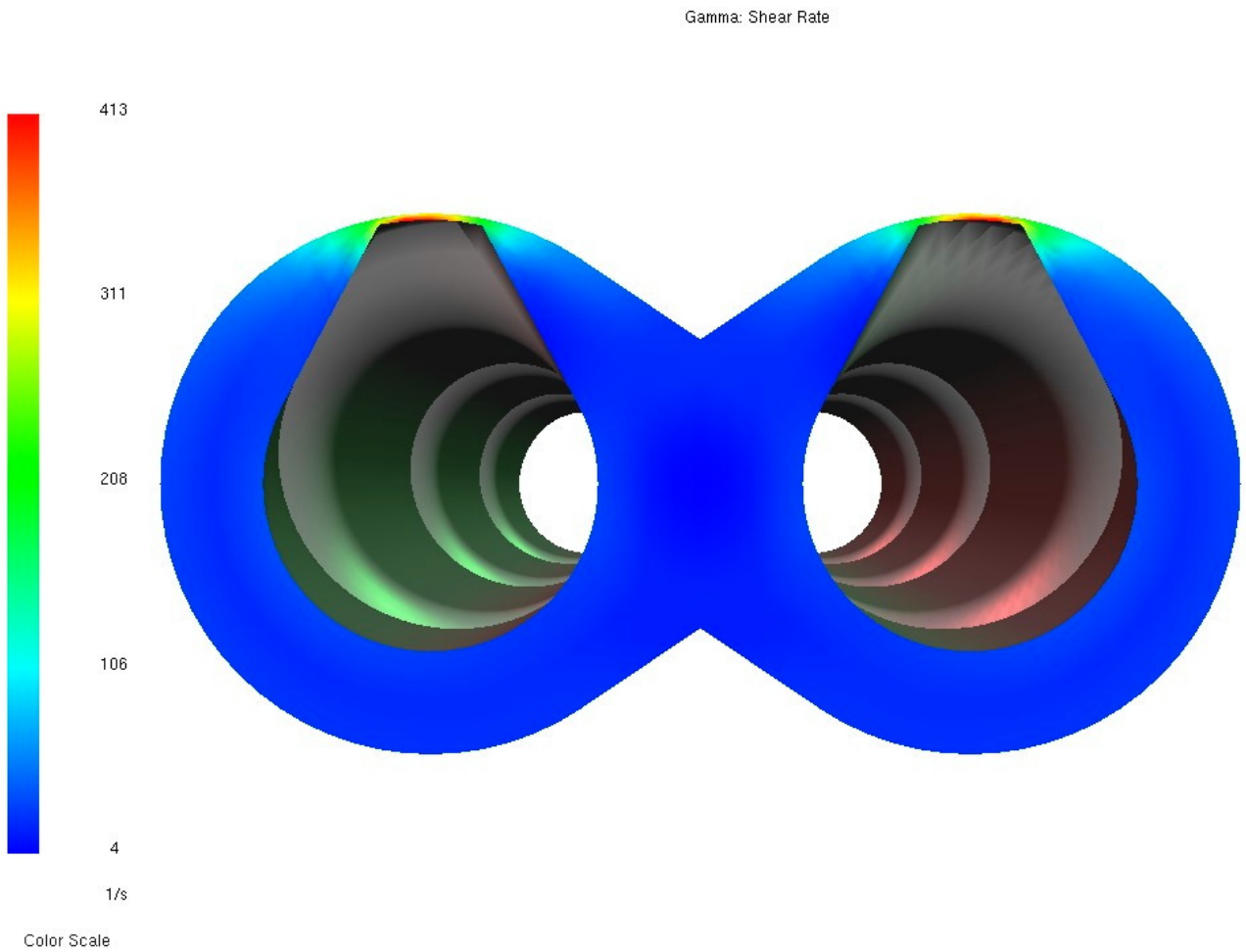

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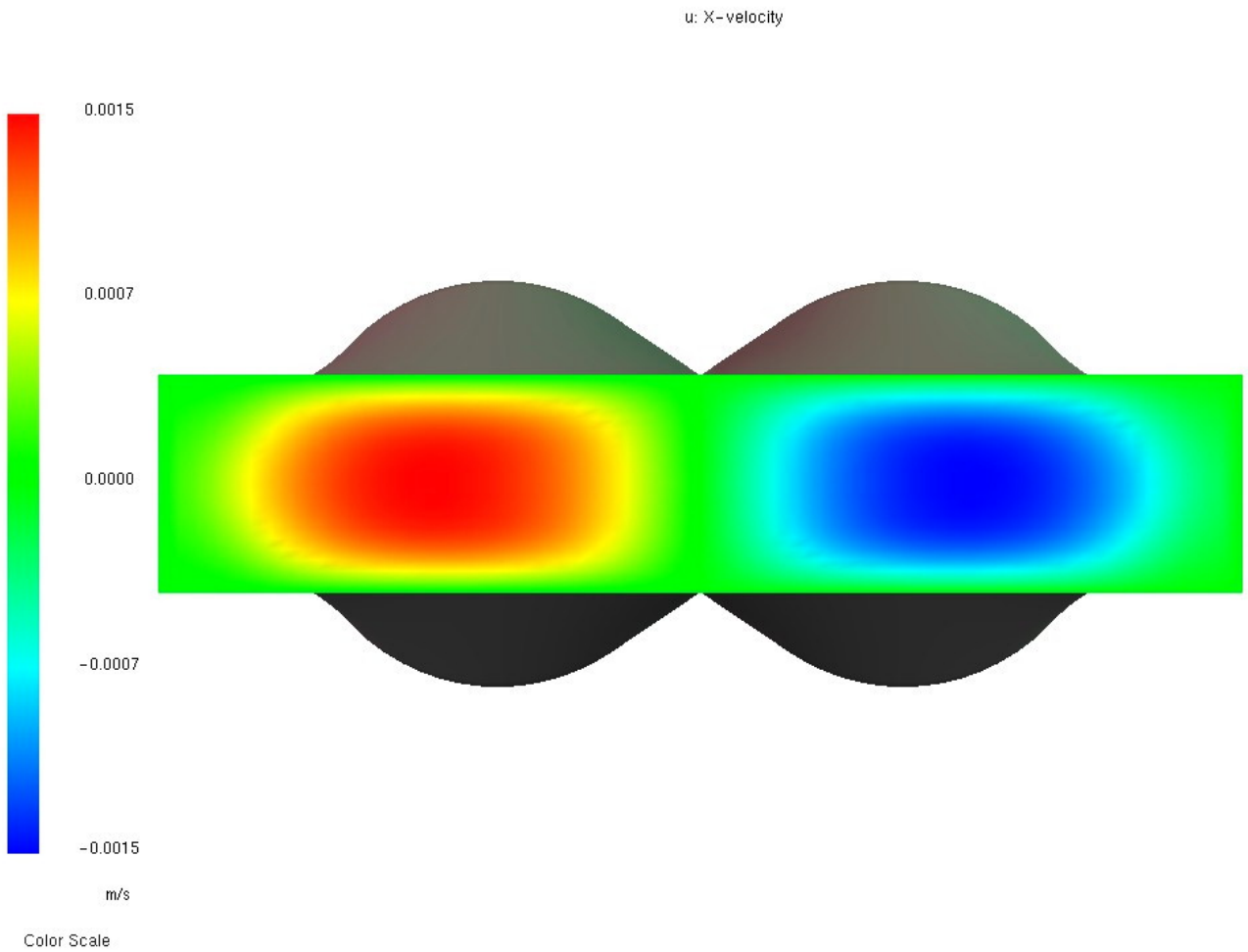

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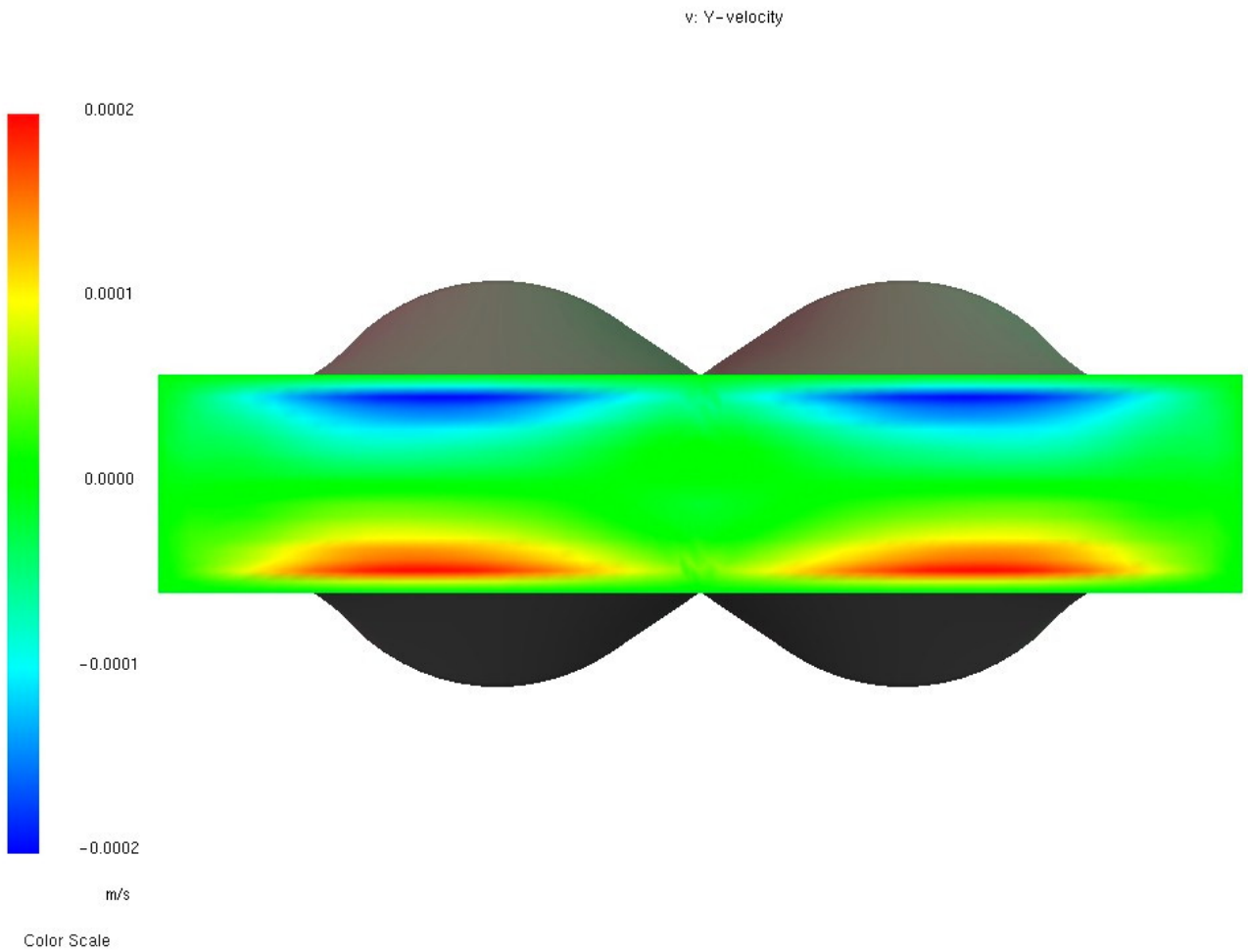

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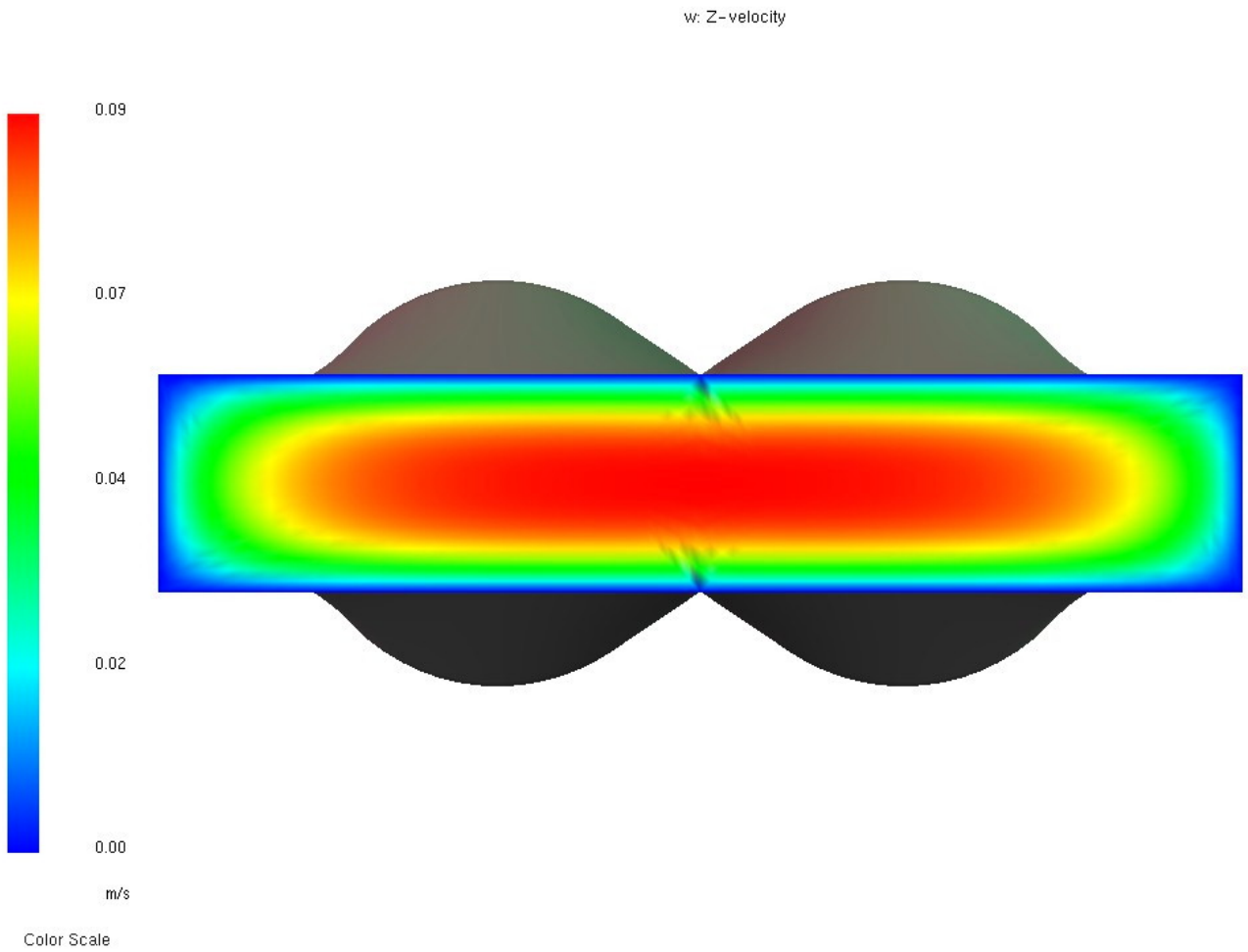

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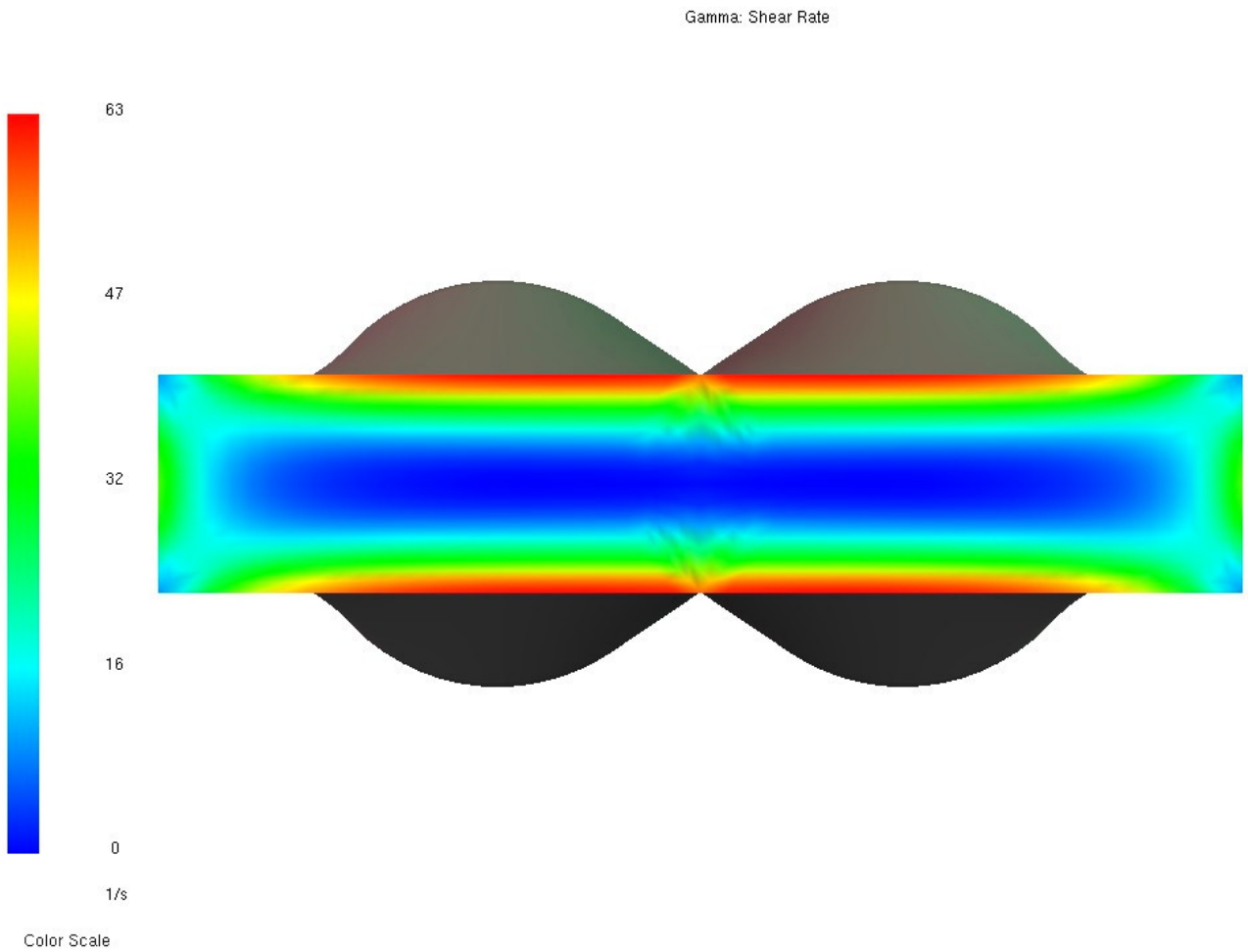

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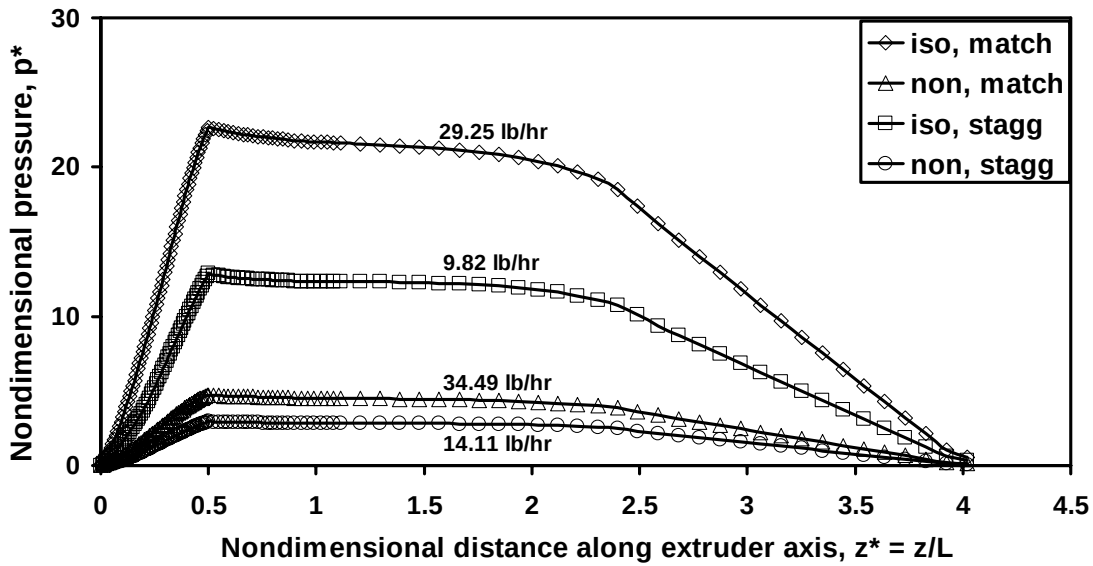
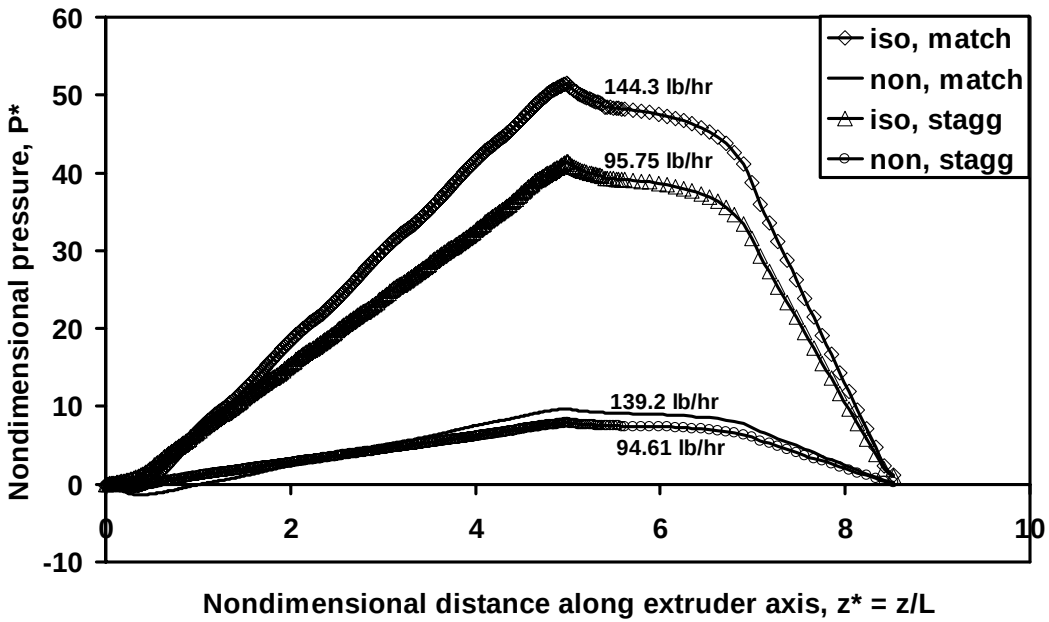


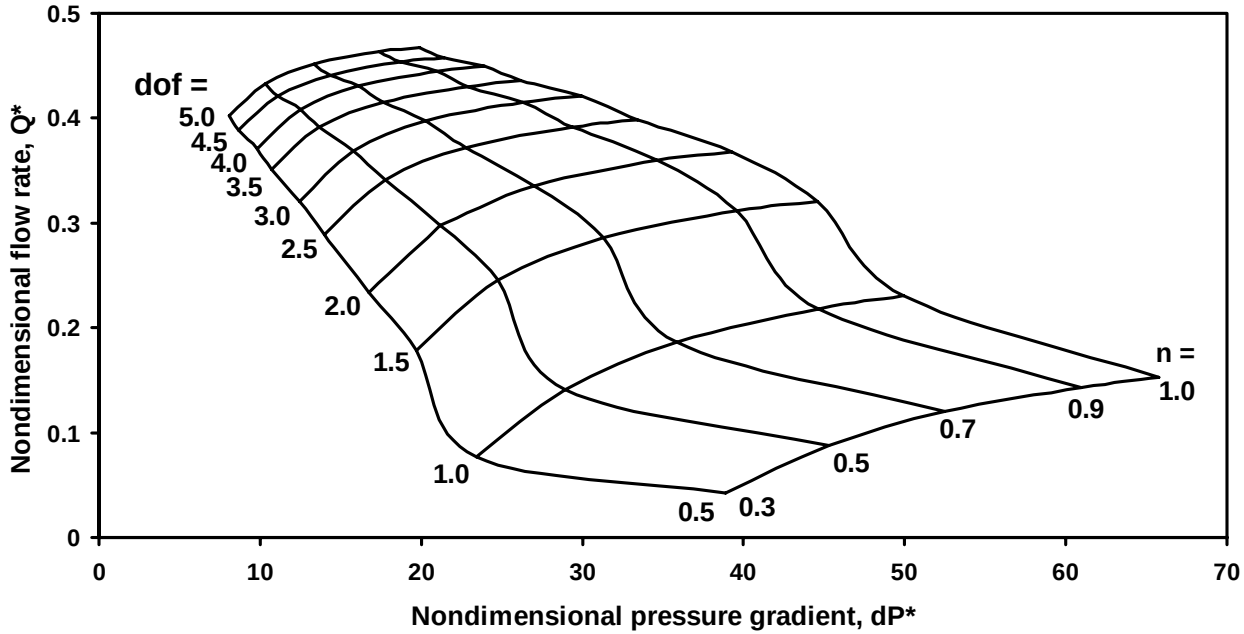
Pressure distribution in CRTTSE-slit die system

dof = 0.5; n = 0.5; N = 100 rpm; $p^* = p/(m_0\omega^n)$



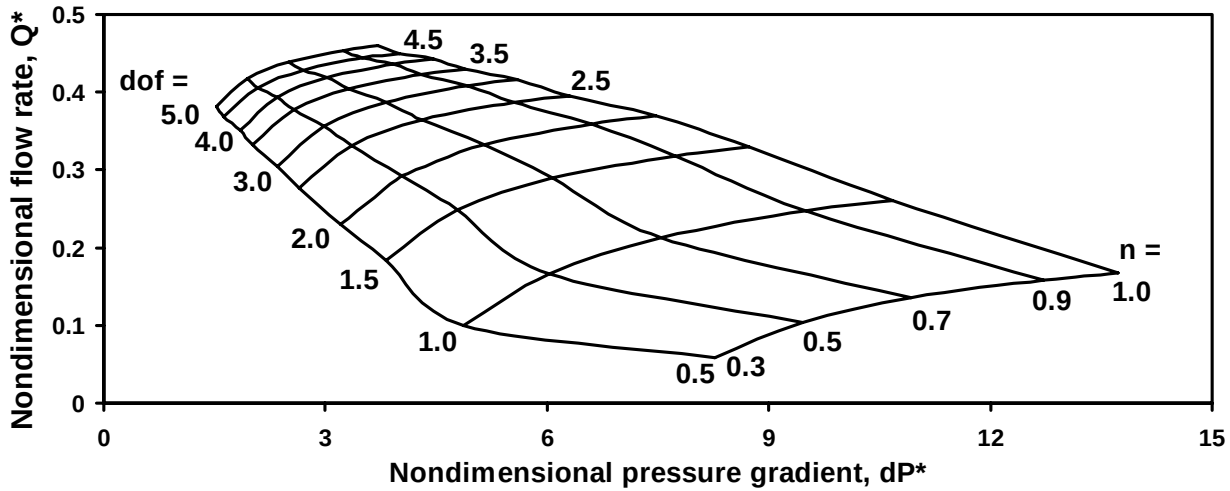
Pressure distribution in the CRTTSE-slit die system

dof = 5.0; n = 0.5; N = 100 rpm; $P^* = P/(m_0\omega^n)$



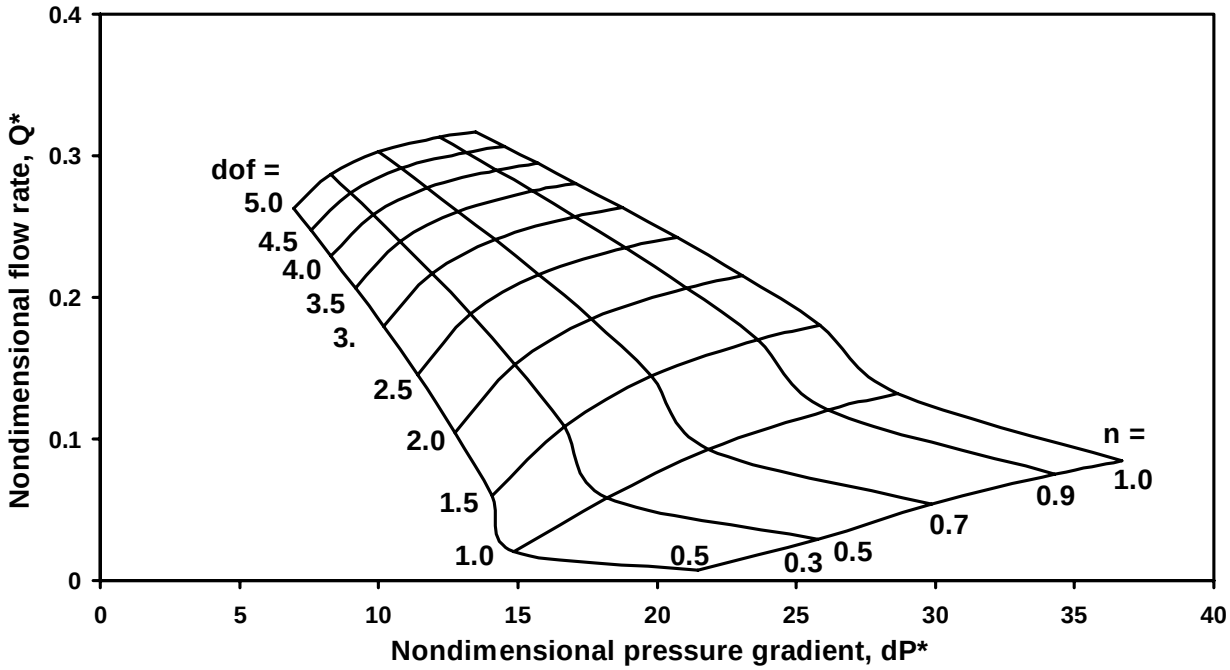
Characteristic curves: Isothermal simulations; Matched flights

N = 100 rpm; $Q^* = Q/(R^3\omega)$; $dP^* = P/(m_0\omega^n dof)$



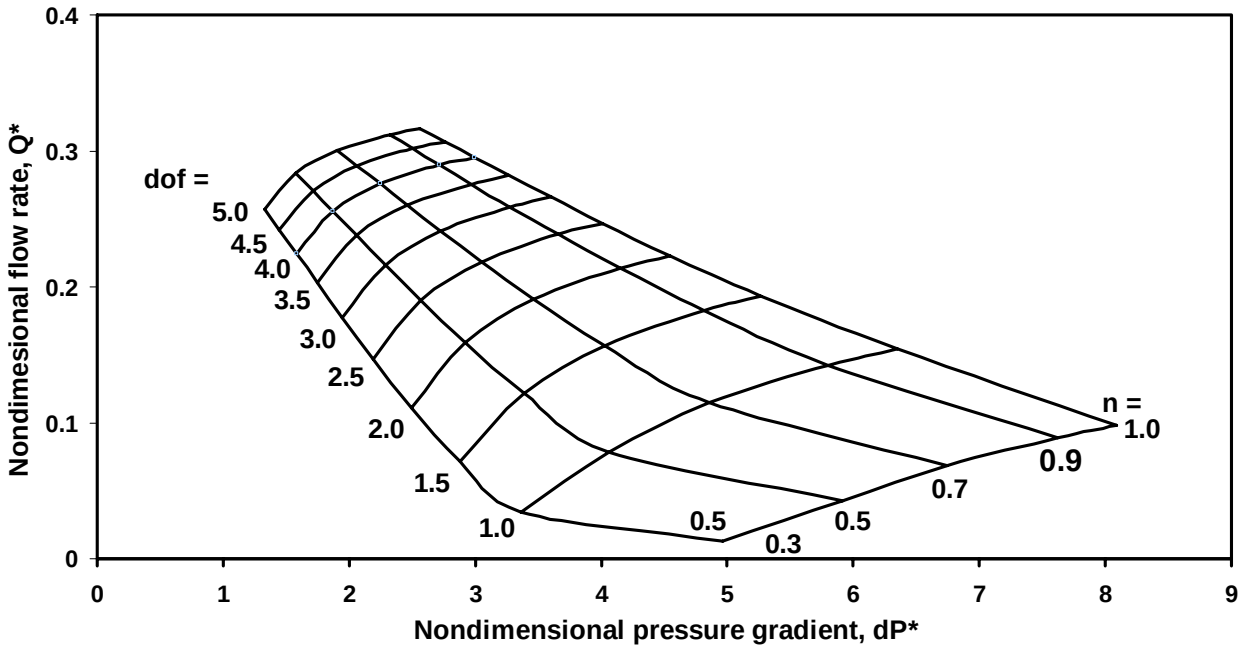
Characteristic curves: Nonisothermal simulations; Matched Flights

N = 100 rpm; $Q^* = Q/(R^3 w)$; $dP^* = P/(m_0 \omega^n dof)$



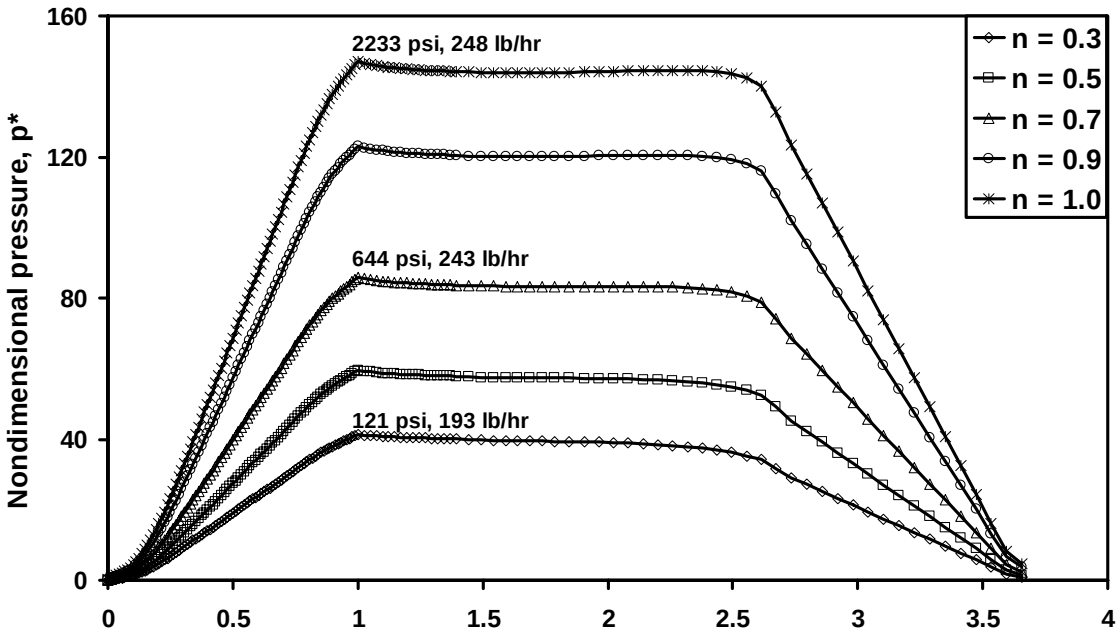
Characteristic curves: Isothermal simulations; Staggered flights

N = 100 rpm; $Q^* = Q/(R^3\omega)$; $dP^* = P/(m_0\omega^n dof)$



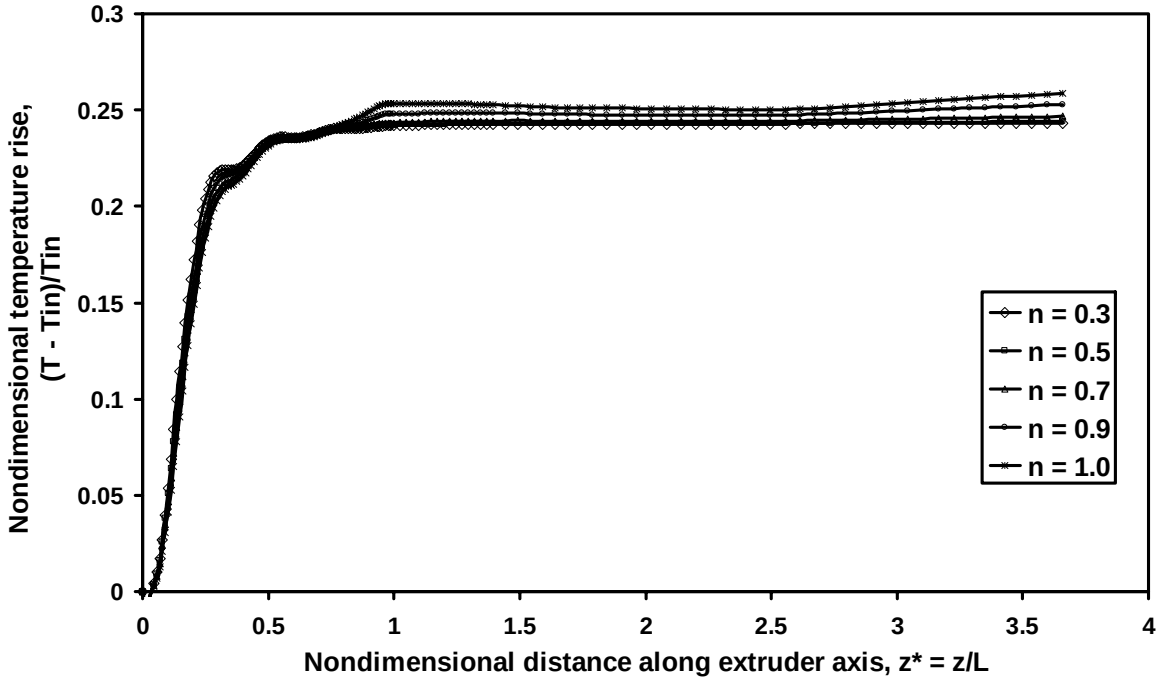
Characteristic curves: Nonisothermal simulations; Staggered flights

N = 200 rpm; $Q^* = Q/(R^3\omega)$; $dP^* = P/(m_0\omega^n dof)$

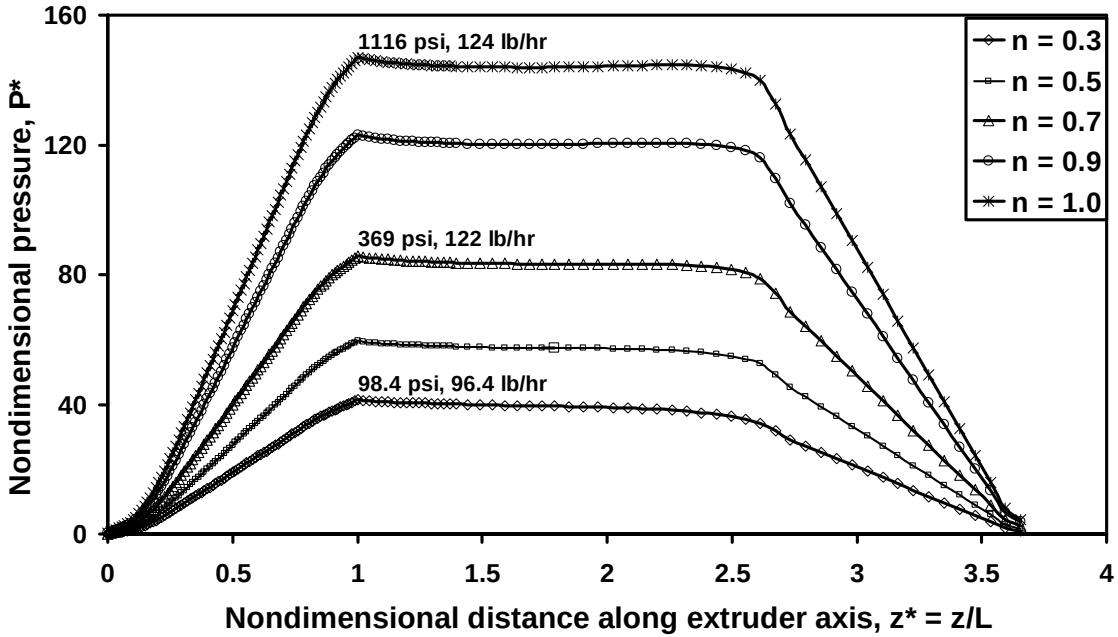


Isothermal pressure distribution in corotating, intermeshing, twin-screw extruder and slit die system

dof = 1; N = 100 rpm; $p^* = p/(m_0\omega^n)$

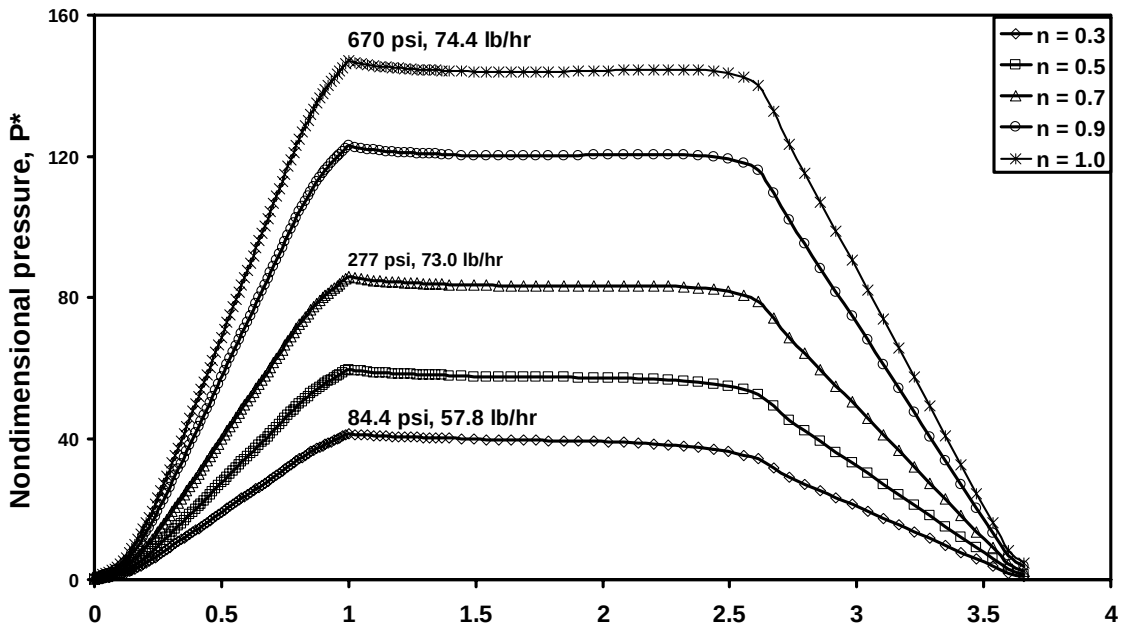


Temperature rise in corotating, intermeshing, twin-screw extruder and slit die system; Isothermal simulations; dof = 1; N = 100 rpm



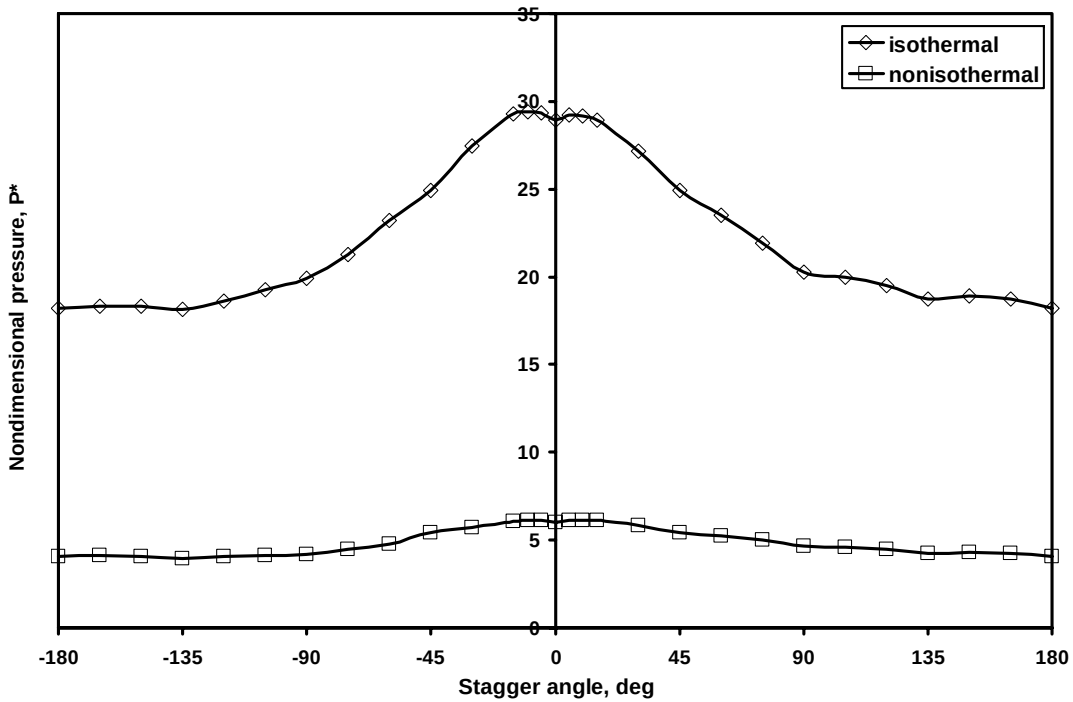
Isothermal pressure distribution in corotating, intermeshing, twin-screw extruder and slit die system

dof = 1; N = 50 rpm; $P^* = P/(m_0\omega^n)$

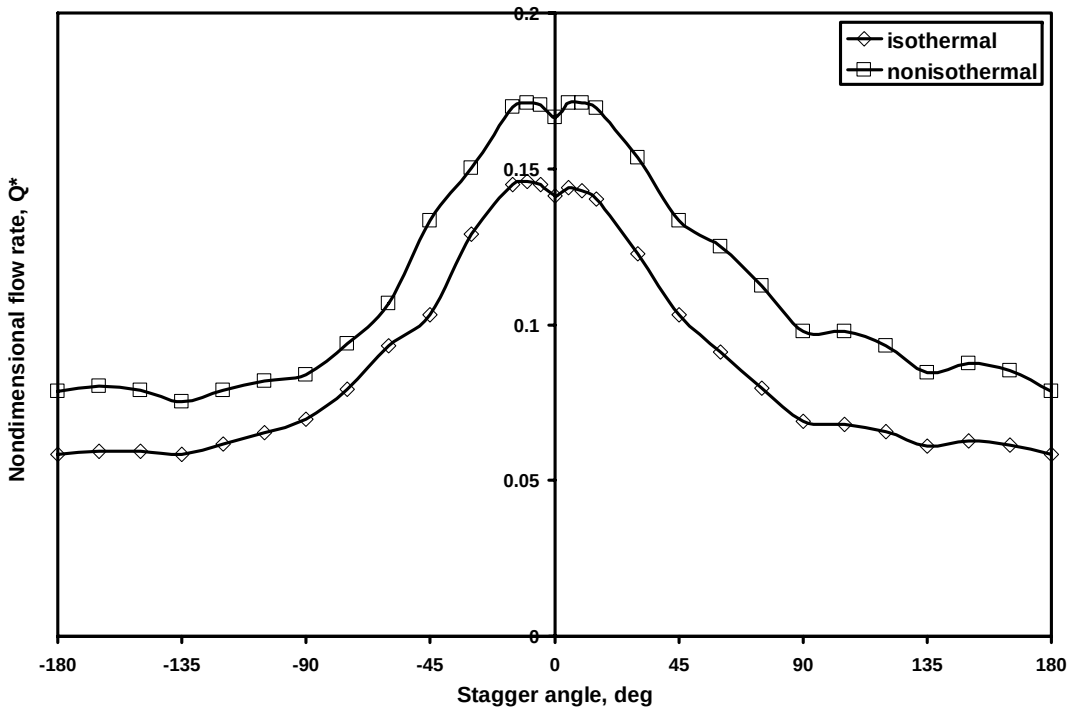


Isothermal pressure distribution in corotating, intermeshing, twin-screw extruder and slit die system

dof = 1; N = 30 rpm; $P^* = P/(m_0\omega^n)$



Nondimensional pressure vs stagger angle
Extruder speed = 100 rpm; Degree of fill = 1; n = 0.5
$P^* = P/(m_0\omega^n)$



Nondimensional flow rate vs stagger angle
Extruder speed = 100 rpm; Degree of fill = 1.0; n = 0.5
$Q^* = Q/(R^3\omega)$

Conclusions

- Every type of extruder comes with its own challenges for modeling
- The methods are generally applicable
- However, the implementation is not straightforward.
- It will be important to prepare for full implementation anticipating that a fully flexible manufacturing platform will be used in the near future.