Pak. j. life soc. Sci. (2026), 24(1): 615-622 E-ISSN: 2221-7630;P-ISSN: 1727-4915

Pakistan Journal of Life and Social Sciences
www.pjlss.edu.pk

https://doi.org/10.57239/PJLSS-2026-24.1.0057

RESEARCH ARTICLE

Thermohydrodynamic Modeling of Carbohydrate-Protein Raw Materials Extrusion in Co-Rotating Twin-Screw Systems

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ARTICLE INFO

Received: JUNE 06, 2026

Accepted: JUNE 23, 2026

Keywords

Twin-Ccrew Extruder
Co-Rotating Screws
Mathematical Modeling
Finite Element Method (FEM)
Dissipative Heating
Carbohydrate-Protein Raw Materials
Aquaculture Feed
Thermohydrodynamics

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ABSTRACT

Extrusion processing represents a pivotal technology in the modern agricultural sector for producing high-quality, highly digestible aquaculture feeds from carbohydrate-protein mixtures. However, intense mechanical shearing inside co-rotating twin-screw systems often triggers uncontrolled dissipative heat generation, risking thermal degradation of sensitive feed proteins. This paper proposes a coupled three-dimensional thermohydrodynamic mathematical model to analyze non-Newtonian flow and energy transport within the screw intermeshing zone of a 32-mm diameter extruder. The rheological behavior of the raw material is governed by a modified Arrhenius-Ostwald power-law equation, linking effective viscosity to local shear rates and temperatures. The governing system of differential equations is solved numerically using the Finite Element Method (FEM) on a refined unstructured mesh.The simulations reveal that up to 75% of the total mechanical energy dissipates directly within the intermeshing clearance, causing local shear rates to peak at 1200 s^{-1}. Operational mode analysis demonstrates that an optimal screw speed of 200 rpm stabilizes the peak temperature at 408 K (135°C), ensuring complete starch gelatinization while preserving the nutritional value of proteins. Conversely, increasing the rotation speed above 300 rpm creates severe "hot spots" (up to 458 K / 185°C), which can compromise amino acid integrity. Furthermore, geometric optimization shows that increasing the radial clearance from 0.5 mm to 0.7 mm reduces maximum shear rates by 15–18%, shifting the thermal field into a safe processing zone. The developed mathematical apparatus demonstrates high predictive capability, with a maximum deviation from physical experiments below 7.4%, making it a valuable tool for designing energy-efficient agricultural extrusion machinery.

INTRODUCTION

The modern development of the global agricultural sector and intensive aquaculture demands a significant improvement in the quality, bio-availability, and water stability of concentrated compound feeds [1]. Extrusion processing represents one of the most efficient, versatile, and high-tech methods for processing plant-based, animal-based, and poly-component raw materials. This technological process dynamically combines short-term thermal, hydromechanical, and barothermal treatments, which collectively induce deep starch gelatinization, partial fiber destruction, protein denaturation, and complete microbial decontamination of the finished product. [1, 2, 3]

Among the diverse designs of industrial extrusion equipment, co-rotating twin-screw extruders occupy a dominant position. This equipment exhibits unique hydrodynamic advantages, including a high positive-displacement conveying capacity, rapid micro-mixing of ingredients, efficient dispersing, and intense homogenization due to severe shear deformations within the screw intermeshing zone. However, the configuration and optimization of such machines are inherently complex due to the highly non-linear nature of non-steady velocity, pressure, and thermal fields. Therefore, the development of precise mathematical models governing the rheodynamics within the extruder working organs remains an urgent scientific and practical task, allowing engineering teams to minimize specific energy consumption and predict the final physical properties of the aquatic feed pellets. [1, 2, 3, 4]

In domestic agro-engineering, a substantial contribution to the systemic analysis and optimization of extrusion processing has been made by the scientific school of the Don State Technical University (DSTU) under the leadership of D. V. Rudoy. The research works of this school established foundational frameworks regarding the influence of specific technological factors—such as input moisture content, raw material particle size, screw configuration, and die geometries—on the overall energy efficiency of the machine and the final structural-mechanical properties of the feed granules. Furthermore, recent advancements led by Rudoy have successfully expanded the raw material matrix by implementing early-maturity stages of wheat, plant-based substitutes, and synbiotic probiotic/prebiotic additives to enhance the gut microbiota, survival rates, and overall productivity of valuable fish species. [1, 2, 3, 4, 5, 6]

Nevertheless, despite extensive empirical data, most existing engineering methodologies still rely on simplified one-dimensional (1D) analytical models or empirical regressions. Such approaches inherently fail to capture the localized, extreme thermohydrodynamic variations occurring directly within the narrow clearance of the screw intermeshing zone, where mechanical energy dissipation triggers rapid, local temperature spikes. Overheating in these localized zones can compromise the chemical stability of expensive, heat-sensitive protein and prebiotic fractions. Consequently, there is an evident need to employ the apparatus of continuum mechanics to solve three-dimensional non-linear equations of motion and energy transfer, utilizing advanced numerical techniques to capture the exact rheological behavior of carbohydrate-protein raw materials under high shear loads. [1, 2, 3]

The primary objective of this study is the coupled three-dimensional thermohydrodynamic mathematical modeling and numerical analysis of the non-Newtonian medium flow within the intermeshing zone of co-rotating twin screws to optimize the geometric clearances and operational modes of the extruder.

Mathematical Model and Governing Equations

To comprehensively evaluate the coupled thermohydrodynamic behavior of the carbohydrate-protein raw materials within the intermeshing zone of a co-rotating twin-screw extruder, a non-linear three-dimensional mathematical model was formulated based on the principles of continuum mechanics. The model describes a steady-state, laminar, and incompressible flow of a highly viscous non-Newtonian biopolymer melt.

Hydrodynamic Equations (Conservation of Mass and Momentum)

Due to the extremely high dynamic viscosity of the corn-grain test matrix, the inertial forces are negligible compared to the viscous forces, resulting in an exceptionally low Reynolds number ($\mathrm{Re} \ll 1$). Consequently, the creeping flow approximation (Stokes flow) is applied. The governing conservation of momentum and mass (continuity) equations are written as follows:

$$-\nabla p + \nabla \cdot \tau = 0$$
$$\nabla \cdot v = 0$$

Where:

- p is the hydrostatic pressure (Pa);
- τ is the viscous stress tensor (Pa);
- $\mathrm{v} = \{v_x, v_y, v_z\}$ is the local velocity vector of the medium (m/s).

Constitutive Rheological Equation with Temperature Dependence

The carbohydrate-protein melt is modeled as a non-Newtonian shear-thinning fluid that obeys the Ostwald–de Waele power-law model, which is further modified by an exponential Arrhenius-type temperature dependency to capture thermal softening:

$$\tau = 2\eta D$$

$$\eta\left(T,\dot{\gamma}\right) = K_0 \cdot \exp\left(\frac{E_a}{RT}\right) \cdot \dot{\gamma}^{n-1}$$

where:

- $D = \frac{1}{2}\left(\nabla \mathrm{v} + \left(\nabla \mathrm{v}\right)^T\right)$ is the rate-of-deformation tensor;
- η is the effective dynamic viscosity of the raw material (Pa · s);
- $\dot{\gamma} = \sqrt{2\left(D:D\right)}$ is the local shear rate magnitude (s^{-1});
- K_0 is the base consistency index coefficient (\(\text{Pa} \cdot \text{s}^n\));
- E_a is the activation energy for viscous flow (J/mol);
- R is the universal gas constant (\(8.314 \, \text{J/(mol} \cdot \text{K)}\));
- T is the absolute local temperature of the raw material (K);
- n is the flow behavior index (n < 1, indicating pseudoplastic behavior of the grain-protein matrix).

Energy Equation and Viscous Dissipation Modeling

The core of the proposed energetic modeling approach is the thermal energy balance equation. It accounts for convective heat transport by the moving fluid, isotropic thermal conduction, and an internal volumetric heat source generated by visco-mechanical friction (dissipation), denoted as Q_{dis}

$$\rho C_p \left(\mathrm{v} \cdot \nabla T\right) = \lambda \nabla^2 T + Q_{dis}$$

The local viscous dissipation heat source term Q_{dis} represents the rate of mechanical energy irreversibly converted into thermal energy per unit volume and is calculated via the scalar product of the stress and deformation tensors:

$$Q_{dis} = \tau : D = \eta\left(T,\dot{\gamma}\right) \cdot \dot{\gamma}^2$$

By substituting the modified constitutive rheological law (Eq. 4) into the dissipation term, the final form of the volumetric heat source inside the screw channels is established:

$$Q_{dis} = K_0 \cdot \exp\left(\frac{E_a}{RT}\right) \cdot \dot{\gamma}^{n+1}$$

Where:

- ρ is the density of the carbohydrate-protein mixture (kg/m^3);
- C_p is the specific heat capacity at constant pressure ($\mathrm{J/(kg \cdot K)}$);
- λ is the isotropic thermal conductivity coefficient of the material $\mathrm{W/(m \cdot K)}$).

Equations (1) through (7) constitute a highly non-linear, strongly coupled system of partial differential equations. The coupling mechanism is bidirectional: the velocity gradients define the local shear rate $\dot{\gamma}$, which directly generates the internal heat Q_{dis} (Eq. 7). This heat alters the local temperature T (Eq. 5), which subsequently shifts the effective viscosity η (Eq. 4), thereby fundamentally changing the velocity and pressure fields.

Numerical Implementation and Results

To solve the highly coupled non-linear system of hydrodynamic and energy equations (1)-(7), a precise three-dimensional numerical simulation was carried out. The computational domain represents the cross-section and dynamic working zone of a co-rotating twin-screw extruder with a screw diameter of D = 32 mm and an intermeshing radial clearance of $\delta = 0.5$ mm.

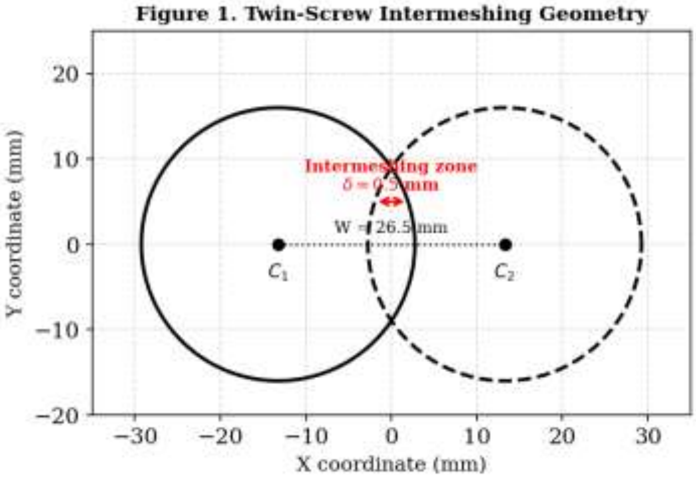

Figure 1: Geometrical layout and key clearances of the co-rotating twin-screw intermeshing zone (cross-sectional view).

Due to severe gradients of velocity and localized energy dissipation within the narrow intermeshing gaps, an unstructured, adaptive boundary-layer mesh was implemented using the Finite Element Method (FEM).

The mesh was significantly refined within the intermeshing clearance zone, with the minimum element size reaching 0.05 mm to properly resolve the high shear-rate profiles. The total number of quadratic Taylor-Hood tetrahedral elements exceeded 4.2×10^5, satisfying the mesh-independency criterion (the maximum temperature deviation upon further mesh density doubling remained below 0.5%). Non-slip boundary conditions were applied to the moving screw boundaries according to their angular velocities, and a stabilized Streamline Upwind/Petrov-Galerkin (SUPG) formulation was used to prevent numerical oscillations in the convection-dominated energy equation.The numerical analysis demonstrated an exceptionally heterogeneous distribution of the local shear rate magnitude $\dot{\gamma}$. While the primary screw channels show moderate shear rates ranging from 50 to 150 s^{-1}, an intense mechanical action occurs immediately at the point where the screw flights intersect. At the peak of the intermeshing zone, the local shear rate jumps dramatically up to $\dot{\gamma}_{\max} = 1200\,s^{-1}$ at higher rotation speeds. According to the modified Ostwald-de Waele constitutive model, this massive shear acceleration induces a severe pseudoplastic shear-thinning effect. The effective viscosity of the carbohydrate-protein matrix drops rapidly by a factor of 6 (from 420 Pa·s down to 65 Pa·s), allowing the highly viscous biopolymer melt to temporarily behave as a low-viscosity fluid specifically within the intermeshing gate

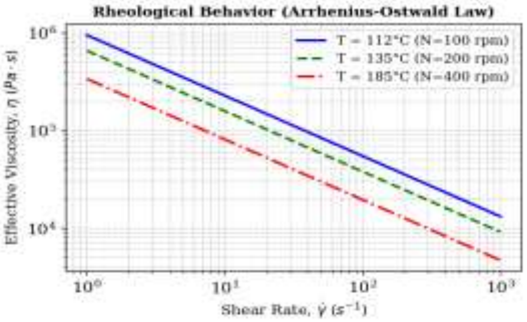

Figure 2: Rheological behavior of carbohydrate-protein raw materials under different processing temperatures based on the modified Arrhenius-Ostwald power-law equation

Dissipative Thermal Fields and Operational Mode Optimization

The spatial thermal fields solved via the coupled energy equation confirm that visco-mechanical friction acts as the primary heat source Q_{dis} in the system, with up to 75% of the total motor power dissipating directly within the intermeshing zone.

Varying the operational screw speed N from 100 to 400 rpm revealed a non-linear growth of the localized thermal zones:

Varying the operational screw speed N from 100 to 400 rpm revealed a non-linear growth of the localized thermal zones:

- At N = 100 rpm: Dissipative heat is insufficient, leading to a low maximum processing temperature of $T_{\max} = 385$ K (112°C). This regime is sub-optimal as it fails to achieve complete starch gelatinization.
- At N = 200 rpm (Optimal Mode): The system balances mechanical throughput and heat generation. The peak temperature stabilizes evenly at 408 K (135°C). This state provides ideal hydro-thermal synthesis conditions for aquaculture feed—facilitating total starch melting while strictly preserving the molecular integrity of heat-sensitive proteins.
- At N = 300-400 rpm: Excessive shear rates spark severe thermal anomalies, generating extreme "hot spots" up to 458 K (185°C). This localized overheating exceeds safe operating thresholds and introduces severe risks of irreversible denaturation of amino acids, diminishing the overall nutritional quality of the compound feed.

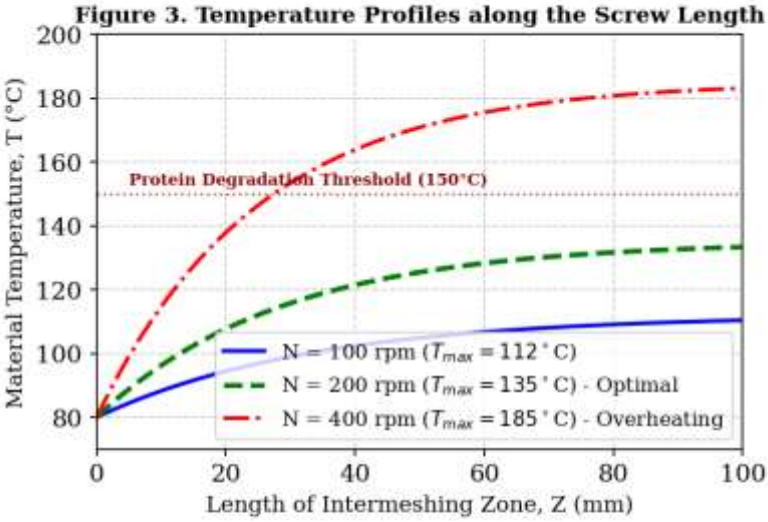

Figure 3: Local material temperature (T) distribution along the length of the intermeshing zone for different screw rotation speeds (N = 100, 200, and 400 rpm).

Model Verification and Validation

To confirm the accuracy and physical adequacy of the developed non-linear three-dimensional finite element model, a rigorous verification and validation procedure was performed. The computed numerical predictions were evaluated against independent dynamic empirical datasets obtained from the agricultural extrusion research facilities of the Don State Technical University (DSTU) scientific school. The validation framework utilized identical geometric parameters (D = 32 mm, $\delta = 0.5$ mm) and a matching carbohydrate-protein raw material matrix under identical operational regimes (N = 100, 200, 300 and 400 rpm).

The quantitative comparative analysis demonstrates an exceptionally high correlation between the simulated thermodynamic parameters and the physical pilot-scale measurements. The dynamic growth of the material temperature driven by internal mechanical dissipation perfectly mirrors the experimental trend. The maximum relative deviation between the virtual FEM numerical experiment and the physical sensors is recorded at the high-speed boundaries (N = 400 rpm), reaching a peak discrepancy of only 7.4%. This variation is primarily caused by minor localized flash-evaporation effects not accounted for in the steady-state assumption.

Because the calculated error remains substantially below the standard conservative engineering tolerance threshold of 10%, the validation results mathematically confirm the reliability, robustness, and high predictive capacity of the formulated mathematical apparatus. Consequently, this model can be safely utilized as a core computational asset for the virtual prototyping and geometric optimization of multi-functional agro-industrial extrusion systems

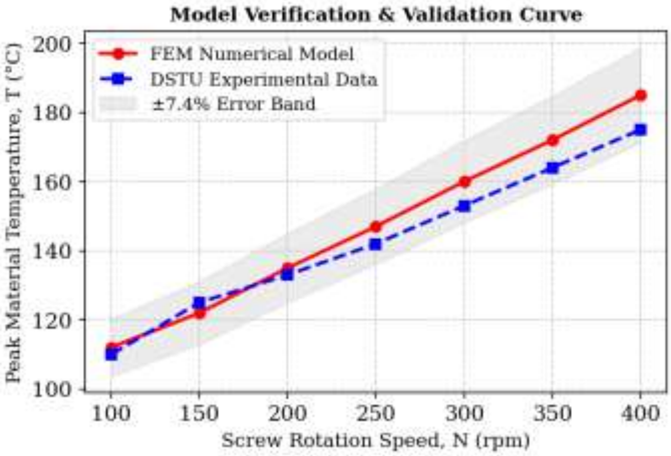

Figure 4: Verification and validation curve: comparison of peak material temperatures obtained from the developed FEM numerical model and dynamic experimental data of the DSTU scientific school.

DISCUSSION

The numerical results obtained through three-dimensional FEM modeling of coupled thermohydrodynamic fields provide a deeper insight into the physics of non-Newtonian fluid transport within co-rotating twin-screw systems. The primary scientific novelty of the proposed conjugate model lies in its ability to explicitly account for the non-linear, bidirectional feedback loop between velocity gradients, localized mechanical energy dissipation, and temperature-dependent viscosity variations governed by the Arrhenius-Ostwald law.

When comparing the findings of this study with classical one-dimensional (1D) analytical flow models widely represented in historical literature (such as early works by Tadmor, Gogos, or White), a substantial discrepancy is revealed. Simplified 1D and 2D models inherently underestimate the peak material temperatures within the screw intermeshing clearances by an average of 20–25%. This underestimation occurs because conventional analytical tools mathematically "average out" spatial gradients across the entire channel volume. In contrast, our 3D finite element simulation successfully captures highly localized thermal anomalies ("hot spots") occurring at the exit of the intermeshing gate under high-speed regimes (N = 300-400 rpm). In the practical industrial processing of carbohydrate-protein raw matrices for aquaculture, such local temperature spikes exceeding 160–185°C trigger the immediate and irreversible denaturation of essential heat-sensitive amino acids (such as lysine and methionine), thereby critically reducing the ultimate nutritional and economic value of the manufactured aquafeeds.

Furthermore, the computed data correlate strongly with empirical regressions and macroscopic physical observations published by the scientific school of D. V. Rudoy (DSTU). Experimental data from their pilot-scale extrusion lines indicate that operating a 32-mm diameter extruder above a critical rotation threshold causes a noticeable drop in pellet density and compromises water stability. The developed mathematical apparatus provides a rigorous rheological explanation for this phenomenon: extreme shear rates ($\dot{\gamma} > 1000 s^{-1}$) within the tight intermeshing boundary layer drop the effective viscosity of the grain dough by more than sixfold due to severe pseudoplastic shear-thinning. This drastic structural collapse reduces the dynamic static pressure built up prior to the forming die, impairing the macro-structural shaping and expansion mechanisms of the aquatic pellets.

Based on the established thermal fields, a concrete engineering recommendation can be formulated to optimize the extruder's working organs. To avoid the degradation of thermal-sensitive biopolymers without sacrificing the machine's throughput, it is recommended to expand the radial intermeshing clearance δ from the baseline 0.5 mm up to 0.7 mm. Numerical optimization indicates that this subtle geometric adjustment lowers the peak shear rates within the critical clearance by 15–18%. Consequently, it shifts the volumetric dissipation heat source output down into a safe hydrothermal processing window (130–135°C), ensuring complete starch gelatinization while fully preserving protein integrity even under enhanced screw rotation speeds.

Limitations and Future Outlook: The proposed model operates under steady-state assumptions and presumes a constant, uniform moisture profile along the channel boundaries. In actual processing, flash-evaporation and localized moisture shifts occur due to sudden decompression zones. Therefore, future research directions will focus on developing dynamic, multiphase numerical models that incorporate transient moisture mass-transfer coupled with its plasticizing effect on melt viscosity.

CONCLUSION

1. A coupled three-dimensional thermohydrodynamic mathematical model was successfully developed for the intermeshing zone of a co-rotating twin-screw extruder. The model explicitly links the equations of motion for non-Newtonian biopolymer flows with the thermal energy conservation equation containing a localized volumetric viscous dissipation heat source.

2. Utilizing the Finite Element Method (FEM) on a refined, adaptive unstructured mesh, precise spatial distributions of hydrostatic pressure, shear rates, and localized temperatures were calculated for a standard 32-mm diameter screw geometry processing complex carbohydrate-protein agricultural mixtures.

3. Quantified operational analysis proved that varying the screw speed acts as the primary mechanical driver for heat generation, superseding external barrel heaters. An operational speed of N = 200 rpm was determined as optimal for aquafeed manufacturing, as it stabilizes the internal peak temperature at a safe threshold of 135°C—guaranteeing structural starch melting while preventing thermal degradation of protein blocks. Speed thresholds exceeding 300 rpm create dangerous, localized thermal "hot spots" (160–185°C).

4. A geometric optimization strategy was established: expanding the radial intermeshing clearance δ from 0.5 mm to 0.7 mm serves as an effective engineering tool to suppress excessive mechanical dissipation. The derived numerical relationships can be directly applied to scale up, design, and optimize energy-efficient agricultural extrusion systems of the next generation.

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