Push or pull, how does silk flow?

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Introduction: The ability to produce artificial silk fibres has **great commercial, industrial and scientific implications.** Silks are multifunctional biopolymers with remarkable mechanical properties, but little is known about how fibres form from a liquid feedstock.[1] Fibrillation occurs due to **a combination of pH change and mechanical shear**. Spider dragline silk proves the most attractive due to its combination of strength, toughness and extensibility (see figure 2).

Figure 1. Major silk producers: Spiders (*N. clavipes*, *upper*) and silkworms (*B. mori*, *lower*)

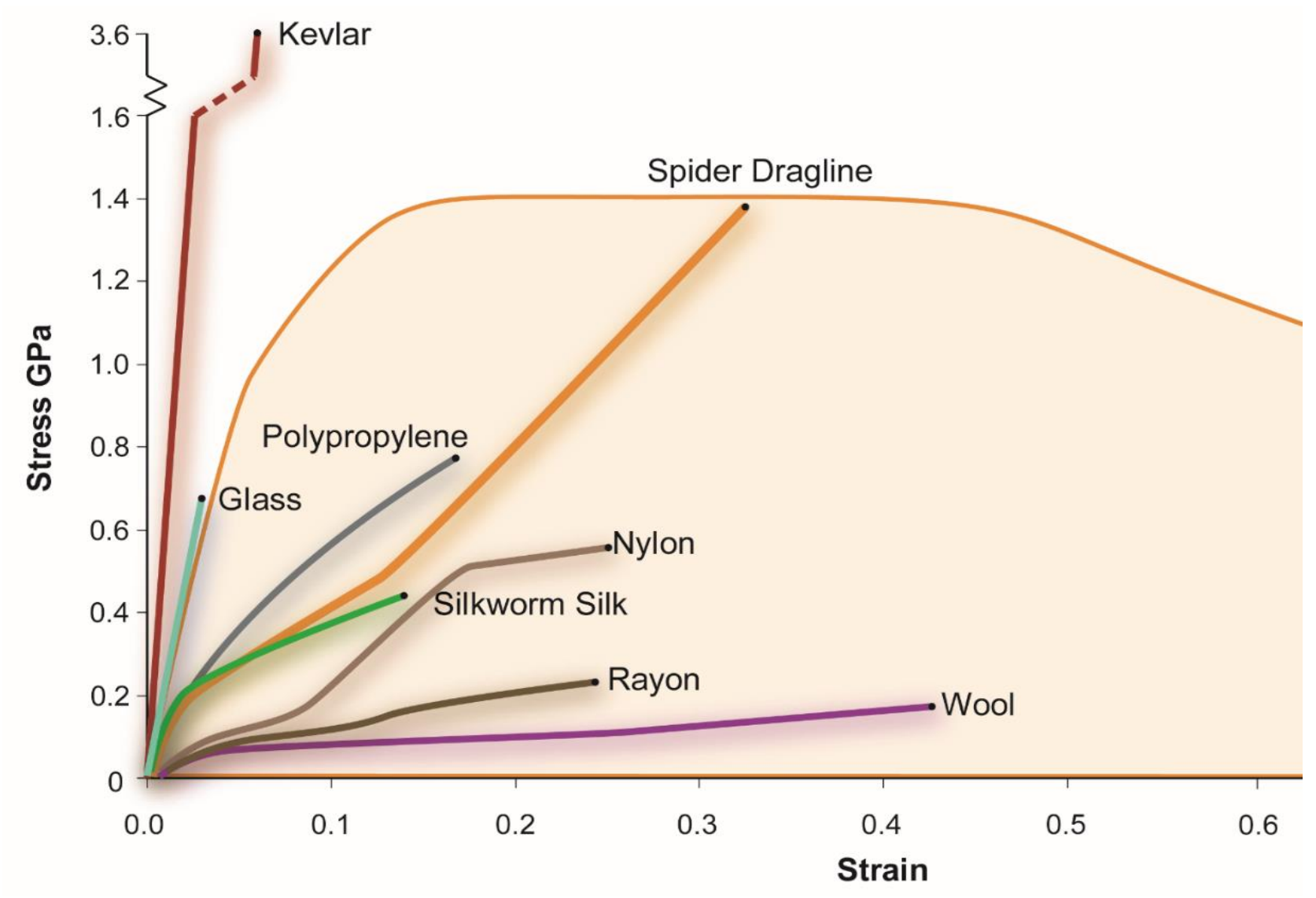

Figure 2. Silk's stress-strain properties. Forced reeling allows access to anywhere in the shaded orange region

Previous attempts to create silk been frustrated by **problems with length, aggregation, and concentration**, with the fibres made proving unremarkable. We believe this is due to not fully understanding Nature's processing methods, and that this is key to successfully handling these wilful proteins.

Our approach involves exploring how die geometry affects the fibres produced, as by understanding the flow conditions **we hope to bring our simulations closer to the natural systems,** which will bring us one step closer to the production of **fibres with tailored mechanical properties**.

Computational Methods: Ducts were modelled as fully parameterised, 2D axisymmetric, single phase laminar flow models, with inlet conditions specified as the pressure required to achieve a specific outlet flowrate (equiv. to spinning rate.)

Rheology: Silk protein solutions have varied rheological properties, but are **shear thinning** and are modelled using the Carreau-Yasuda model[2]:

$$\eta(\dot{\gamma}) = \eta_{\infty} + (\eta_0 - \eta_{\infty})(1 + (\lambda\dot{\gamma})^a)^{\frac{n-1}{a}}$$

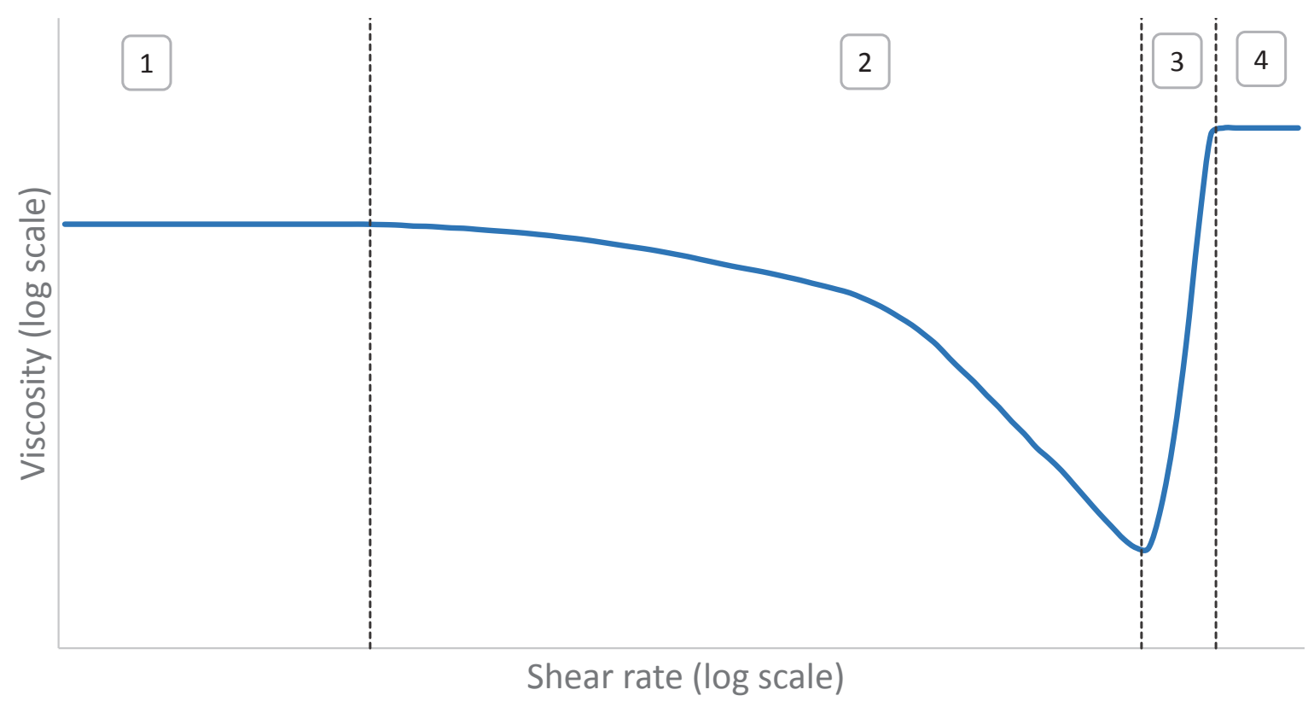

Figure 3 – Silk's shear ramp response: 1 – Pseudo-Newtonian; 2 – Shear thinning; 3 – Fibrillation; 4 – Viscoelastic solid.

Geometry: Ducts are modelled by fitting curves to previously dissected glands, and as exponential, parabolic and linear tapers to a range of outlet diameters.

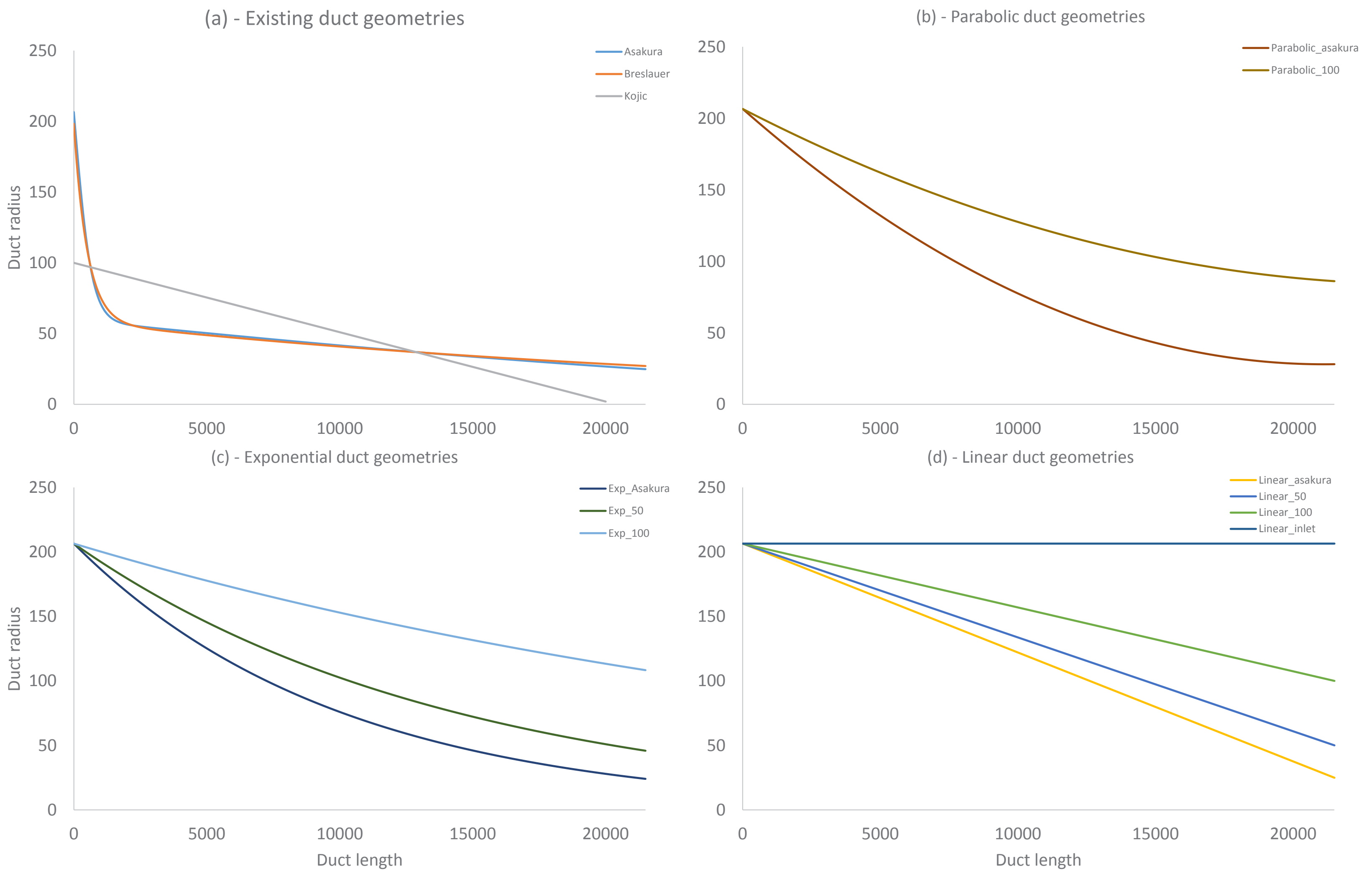

Figure 4. Ducts were modelled with a wide range of taper styles. The existing duct geometries (a), were compared with parabolic (b), exponential (c) and linear (d) geometries. Note the inclusion of the limiting case of a zero taper in panel (d).

Previous work: Previous attempts to model silk flow have failed to align pressure and spinning speed, with realistic internal pressures suggesting nanometre rates of production, while realistic spinning speeds require an internal pressure several orders of magnitude higher than that which would rupture a silkworm! (see figure 5). The difficulties of the problem are exacerbated by the wide range of viscosities exhibited by silkworm dopes[3], all of which are considered to be viable feedstocks (see figure 6), and further compounded by the complexity of the geometry to be emulated, which can be seen on the right in figure 7[4].

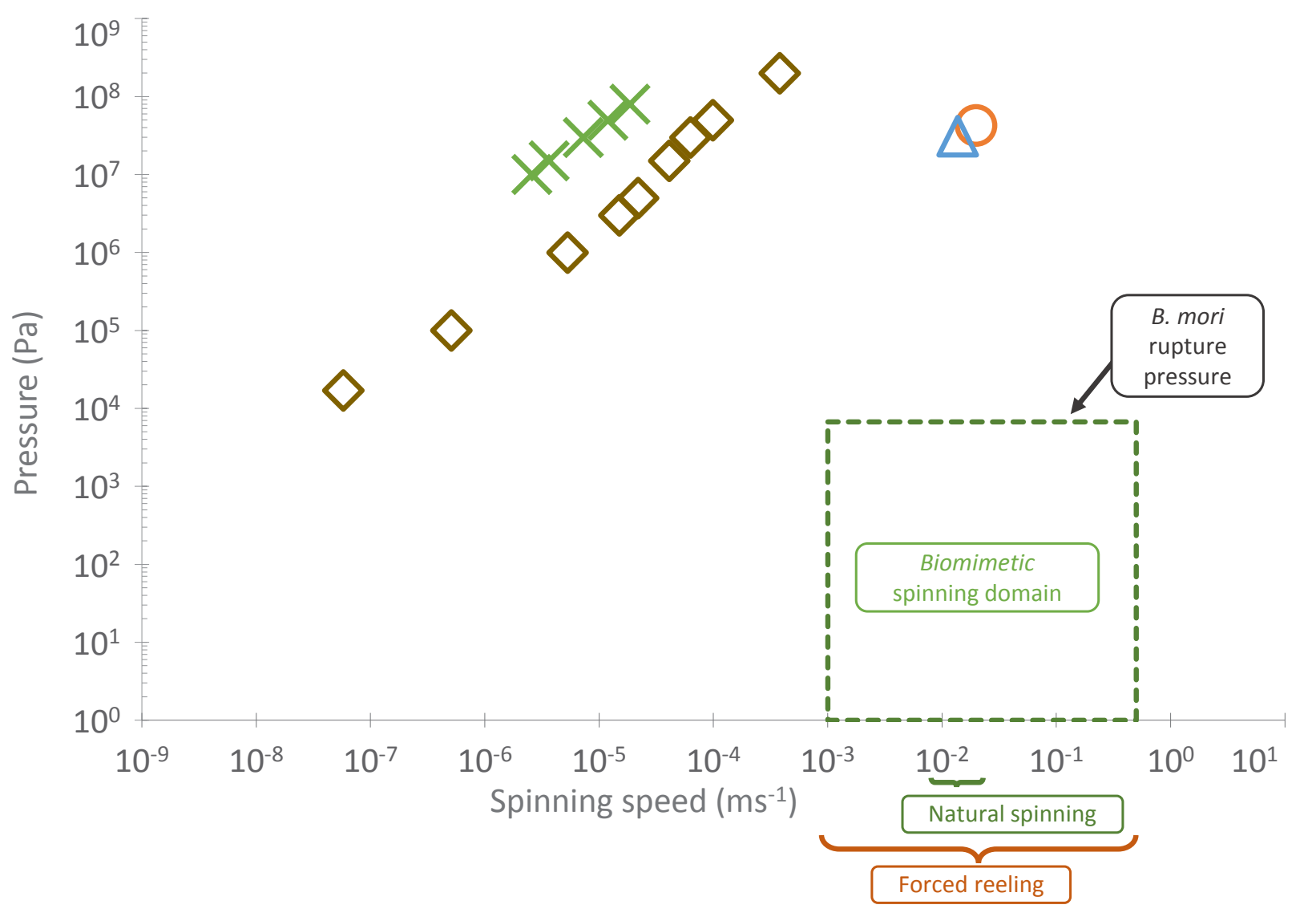

Figure 5. Previous estimations of pressure requirements lie well outside the biomimetic spinning domain

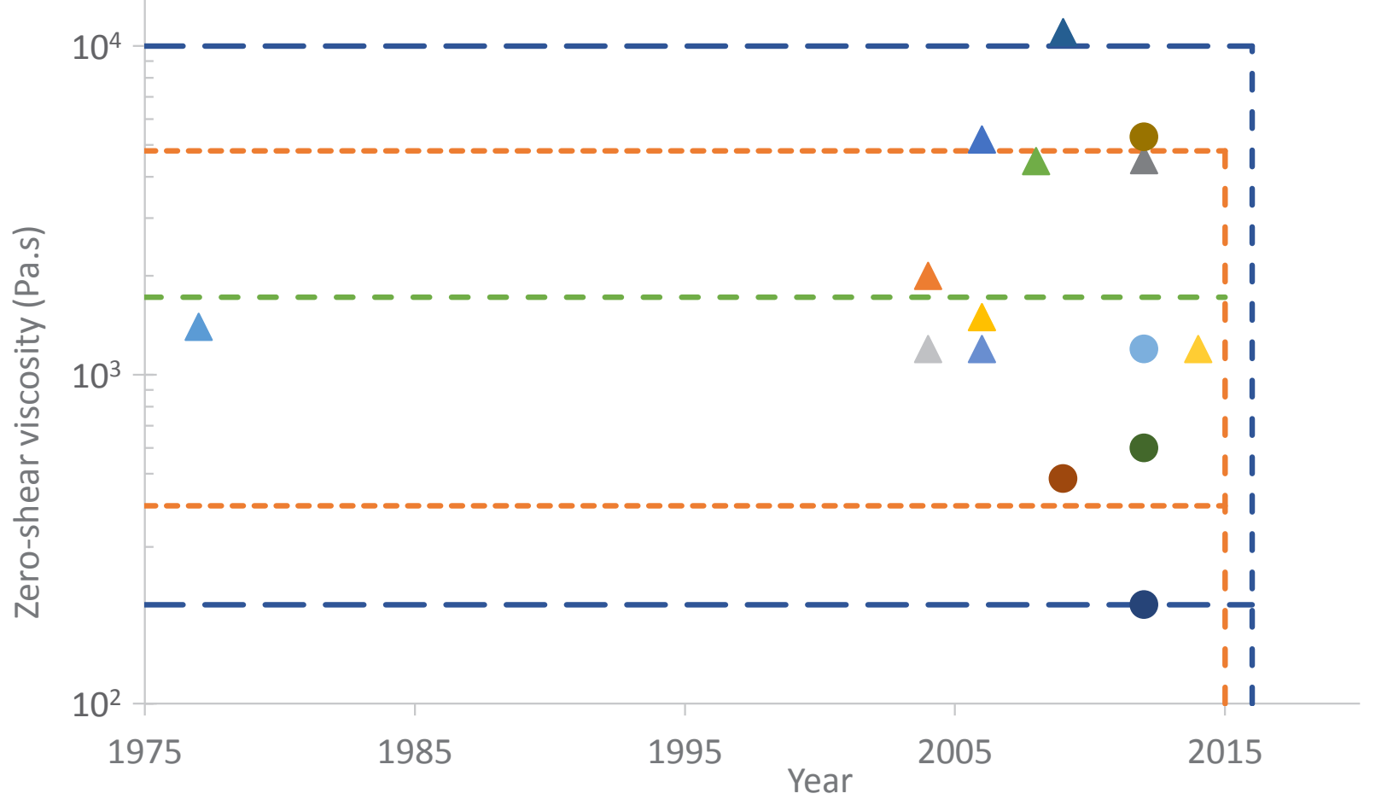

Figure 6. Wild (circles) and domesticated (triangles) dopes, 2015 range (orange), mean (green); and 2016 (blue).

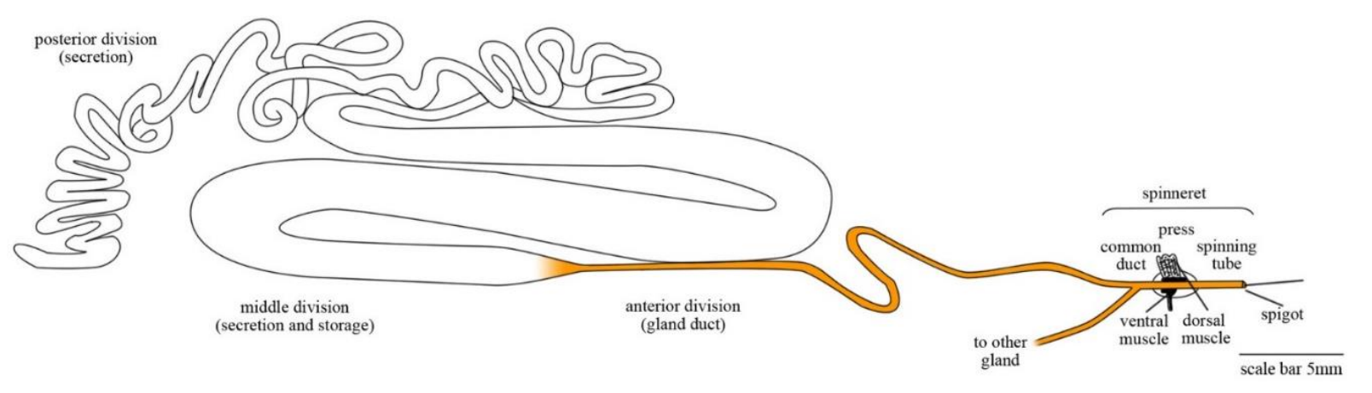

Figure 7. One of the two glands in the *B. mori* silkworm

Results: Pressure requirements can be reduced by lowering both taper severity and increasing outlet diameter. However this is unrepresentative of the natural system and even the limiting case proves insufficient to enter spinning domain.

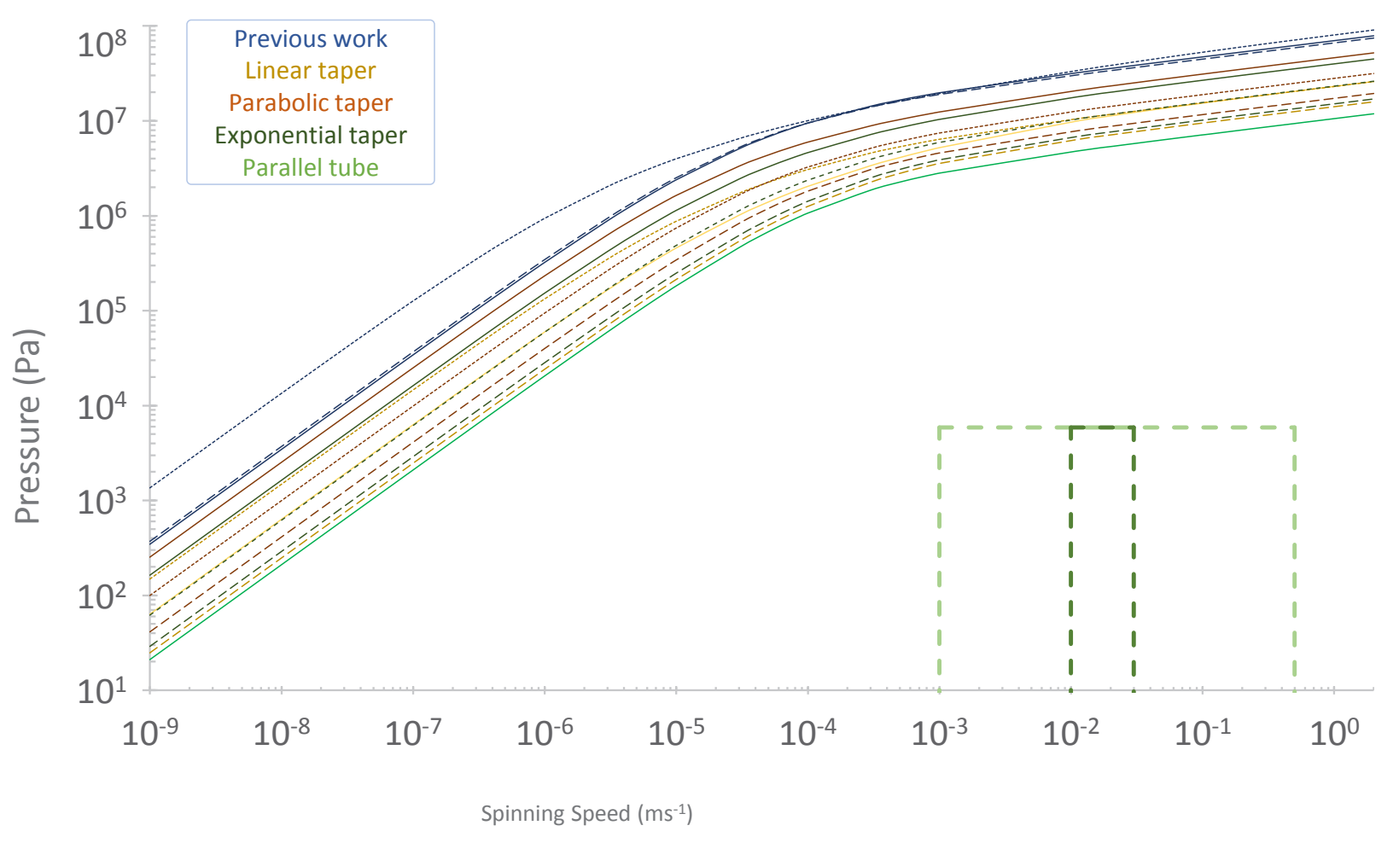

Figure 8 : reducing taper severity/extent reduces pressure needs

Lowering zero shear viscosity reduces pressure requirements, but greatest effect comes from reducing wall friction. Assuming no drag allows lowest reported zero shear viscosity to enter spinning domain, but not the full range (all of which are viable feedstocks).

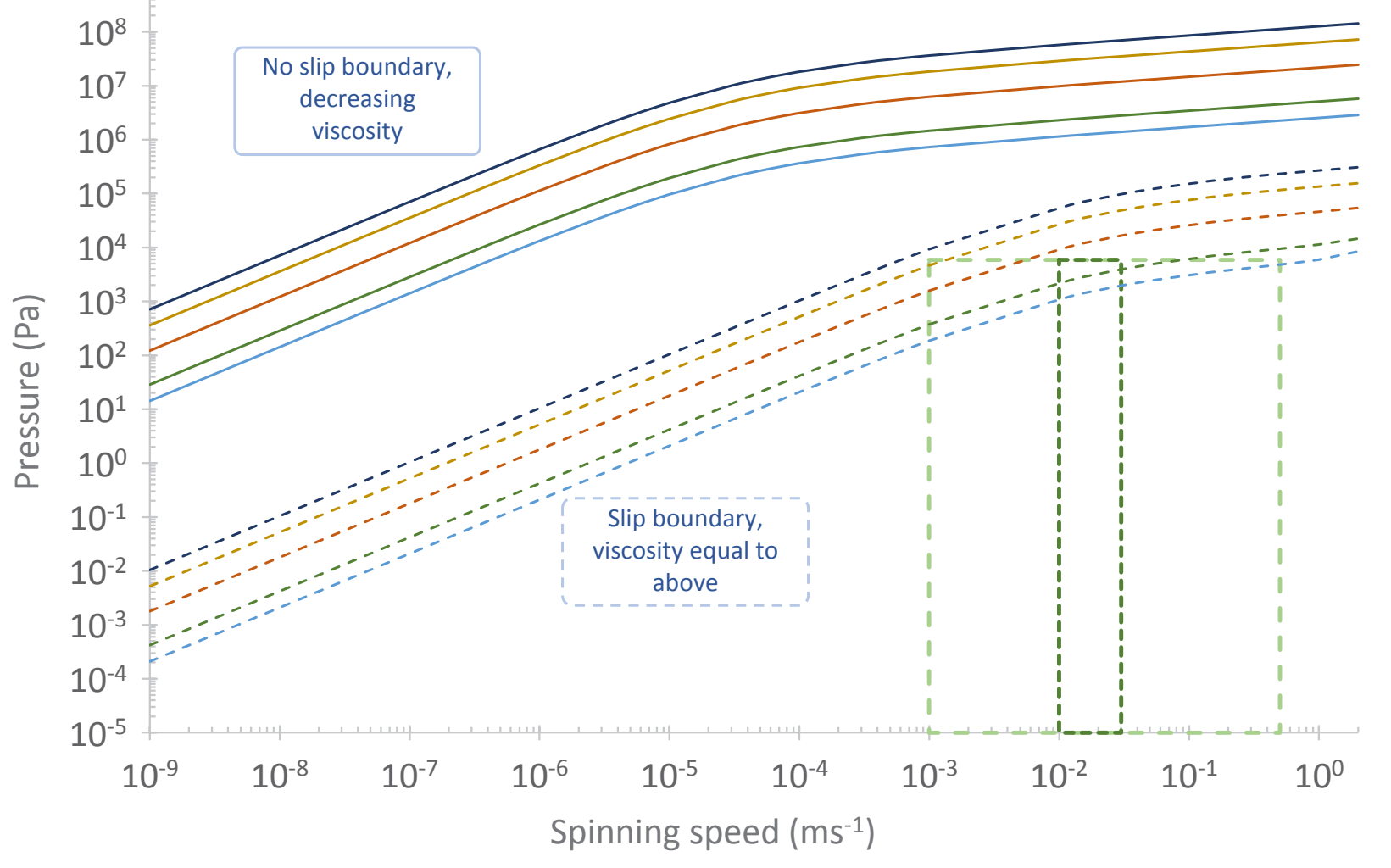

Figure 9 : reducing zero shear viscosity and/or wall friction reduces pressure needs

If we assume fluids are immiscible, plug flow allows modelling as a single phase consisting of lubricant. Using secondary proteins as lubricant is insufficient, yet water (major solvent in the system[5]) can reach parts of the spinning domain.

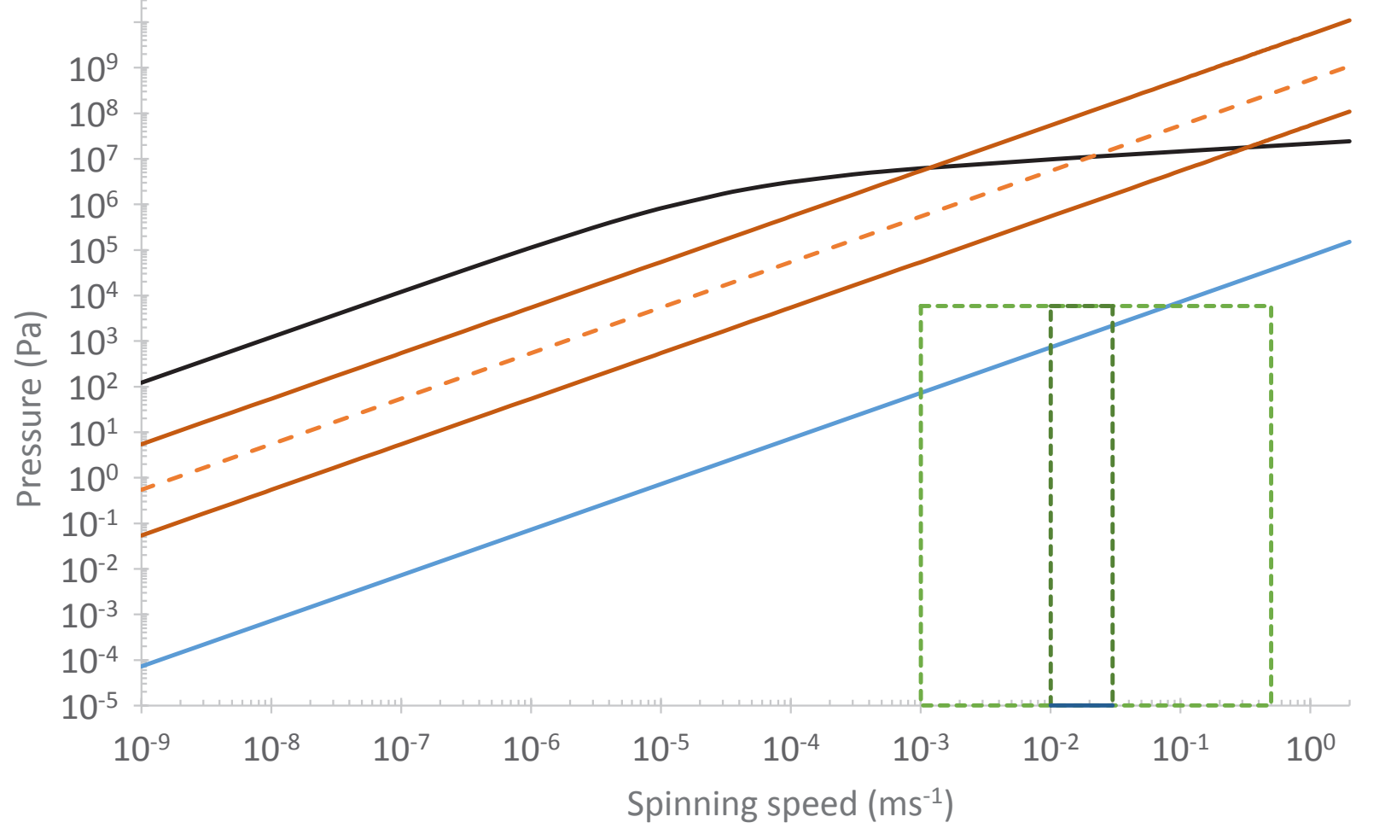

Figure 10: changing the working fluid to solvent allows partial entry to biomimetic spinning domain

Conclusions: Better rheological data and models have closed the gap between simulated and natural domains, but that they remain separate suggests that **silk production is unlikely to be an extrusion process.** To confirm this, we need to characterise the other fluids in the gland, then develop multiphase flow models.

References:

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