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Modeling of straight jet dynamics in electrospinning of polymer nanofibers

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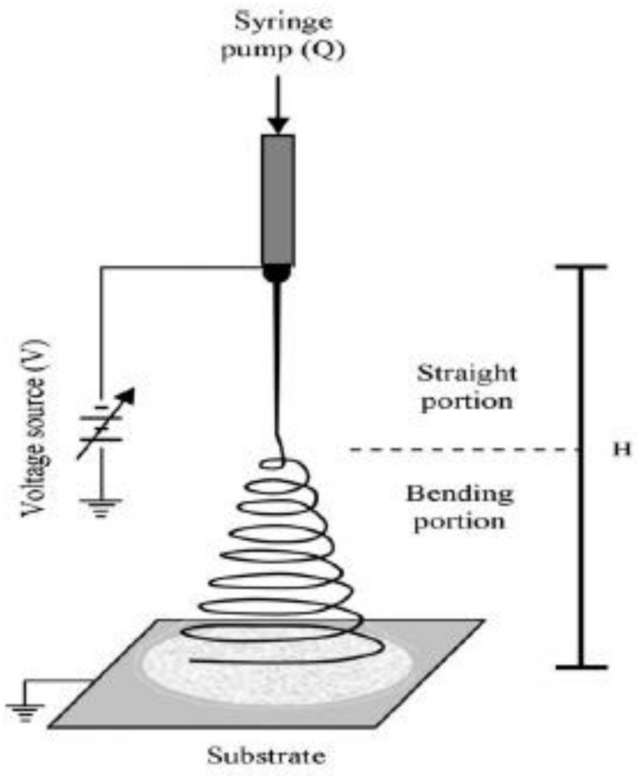
Introduction

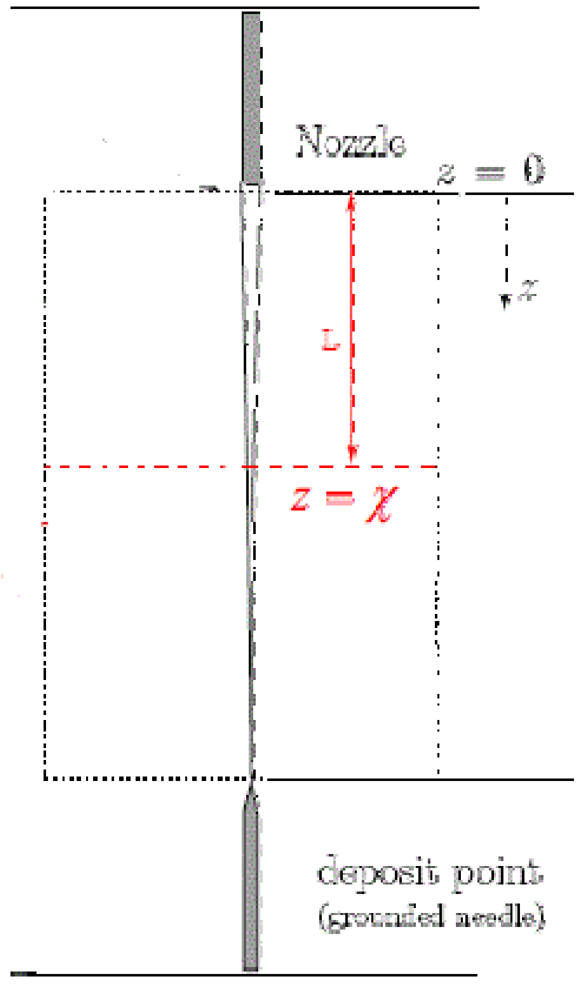
- Nanofibers are produced by solidification of a polymer solution stretched by an electric field.
- Properties:
  - High surface area per unit mass,
  - Very high porosity,
  - Layer thinness,
  - High permeability,
  - Low basic weight,
- Applications:
  - wound dressing,
  - drug or gene delivery vehicles, biosensors,
  - fuel cell membranes and electronics,
  - tissue-engineering processes.



Mathematical modeling in electrospinning process of nanofibers: a detailed review- S. Rafiei, S. Maghsoodloo, B. Noroozi, Mottaghitalab and A. K. Haghi(2012)

Objective

- Build a mathematical model to predict the **radius** of a straight jet electrospinning process.
- Validate the model for
  - Newtonian fluid
  - Non Newtonian fluid
  - Viscoelastic fluid
- Study the dependence of radius on various working parameters.



Basic Assumptions

- Slender body theory
  - $R(z) \propto z^{-1/4}$
  - $R + 4zR' = 0$
- Leaky dielectric model
  - Free charge which accumulates on the interface modifies the field.
  - Viscous flow develops - stresses balance the tangential components of the field acting on interface charge
- Laminar flow
- Electric field inside the fibre is being solved

D. A. Saville, Electrohydrodynamics: The Taylor-Melcher Leaky Dielectric Model

Mathematical Model

- Mass conservation equation:
  - $\pi R^2 v = Q$
- charge conservation equation:
  - $\pi R^2 KE + 2\pi R v \sigma = I$
- Electric Field equation:
  - $E(z) = E_\infty(z) - ln\chi\left(\frac{1}{\bar{\epsilon}}\frac{d(\sigma R)}{dz} - \frac{\beta}{2}\frac{d^2(ER^2)}{dz^2}\right)$
- Momentum Equation:
  - $\frac{d(\pi R^2 \rho v^2)}{dz} = \pi R^2 \rho g + \frac{d[\pi R^2(-p+\tau_{zz})]}{dz} + \frac{\gamma}{R} 2\pi R R' + 2\pi R(t_t^e - t_n^e R')$

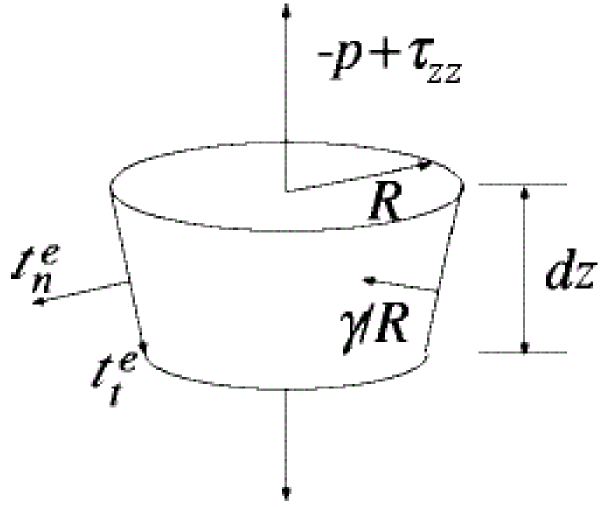


FIG. 1. Momentum balance on a short section of the jet.

J.J. Feng, Phys. Fluids 14 (2002) 3912–3926

Scaling

Characteristic Scales

Length: R_0

Velocity: $v_0 = Q/(\rho R_0^{2})$

Electric field: $E_0 = I/(\rho R_0^{2} K)$

Surface charge density: $\sigma_0 = \bar{\epsilon} E_0$

Stress: $\tau_0 = \eta_0 v_0 / R_0$

Dimensionless groups:

Froude number: $Fr = \frac{v_0^2}{gR_0}$,

Reynolds number: $Re = \frac{\rho v_0 R_0}{\eta_0}$,

Weber number: $We = \frac{\rho v_0^2 R_0}{\gamma}$,

Deborah number: $De = \frac{\lambda v_0}{R_0}$,

viscosity ratio: $r_\eta = \frac{\eta_p}{\eta_0}$,

aspect ratio: $\chi = \frac{L}{R_0}$,

Electric Peclet number: $Pe = \frac{2\bar{\epsilon} v_0}{K R_0}$,

Electrostatic force parameter: $\varepsilon = \frac{\bar{\epsilon} E_0^2}{\rho v_0^2}$,

Dielectric constant ratio: $\beta = \frac{\epsilon}{\bar{\epsilon}} - 1$,

Mathematical Model (non-dimensional)

- Mass conservation equation:
  - $R^2 v = 1$
- Charge conservation equation:
  - $ER^2 + PeRv\sigma = 1$
- Electric Field equation:
  - $E = E_\infty - ln\chi(\frac{d(\sigma R)}{dz} - \frac{\beta}{2}\frac{d^2(ER^2)}{dz^2})$
- Momentum Equation:
  - $vv' = \frac{1}{Fr} + \frac{T\prime}{ReR^2} + \frac{R\prime}{WeR^2} + \varepsilon(\sigma\sigma' + \beta EE' + \frac{2E\sigma}{R})$

Tensile Force,

$T = 3\eta R^2 v'$, for Newtonian and Non-Newtonian

$T = T_p' + 3\eta(1 - r_\eta)R^2 v'$, for viscoelastic fluids.

Polymer Stress Tensor Equation (Giesekus viscoelastic fluid)

$$\tau_{prr} + \lambda(v\tau'_{prr} + v'\,\tau_{prr)} + \alpha\frac{\lambda}{\eta_p}\tau_{prr}{}^2 = -\eta_p v'$$

$$\tau_{pzz} + \lambda(v\tau'_{pzz} - 2v'\,\tau_{pzz)} + \alpha\frac{\lambda}{\eta_p}\tau_{pzz}{}^2 = 2\eta_p v'$$

Non-dimensionalised form

$$\tau_{prr} + De(v\tau'_{prr} + v'\,\tau_{prr)} + \alpha\frac{De}{\eta_p}\tau_{prr}{}^2 = -r_\eta v'$$

$$\tau_{pzz} + De(v\tau'_{pzz} - 2v'\,\tau_{prr)} + \alpha\frac{De}{\eta_p}\tau_{pzz}{}^2 = 2r_\eta v'$$

Boundary Conditions

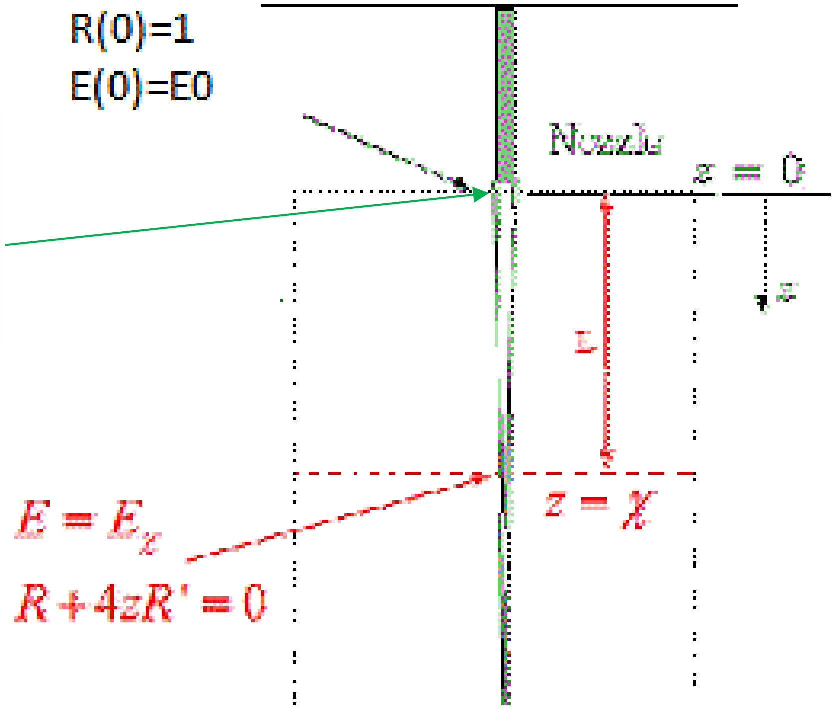
Model is solved for

- 1-D geometry
- R is converted to v using the mass balance equation and then solved

- Mathematics ODE solver is used

$$\tau_{prr} = 2r_\eta \frac{R'}{R^3}$$

$$\tau_{pzz} = -2\tau_{prr}$$

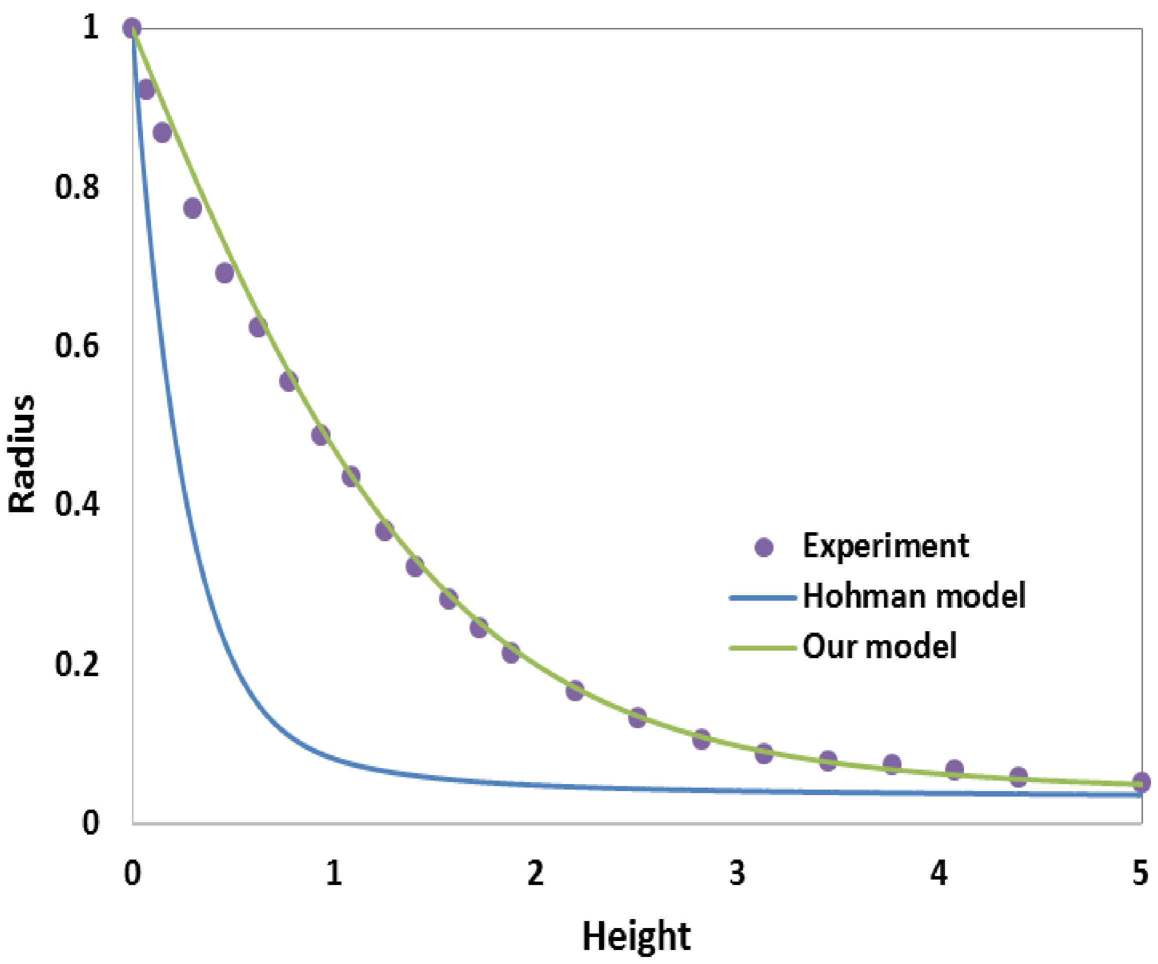


A Model for Electrospinning Viscoelastic Fluids, P.C. Roozemond, 0576690 Report No. MT07.12

Results

- Experimental data of Hohman *et al.* for a glycerol jet
  - R_0=0.08 cm, L=56 cm, Q=1 mL/min, E_∞= 5 kV/cm, I=170 nA, kinematic viscosity=514.9 cm2/s, *K*=50.01 mS/cm
- The parameters of Hohman *et al.*:
  - *X=75*, B=45.5, Re=$4.451*10^{-3}$, We=$1.099*10^{-3}$, Fr=$8.755*10^{-3}$, Pe=1.835310^{-4}, ε=0.7311, E_∞=5.914, K=0.01 µS/cm.

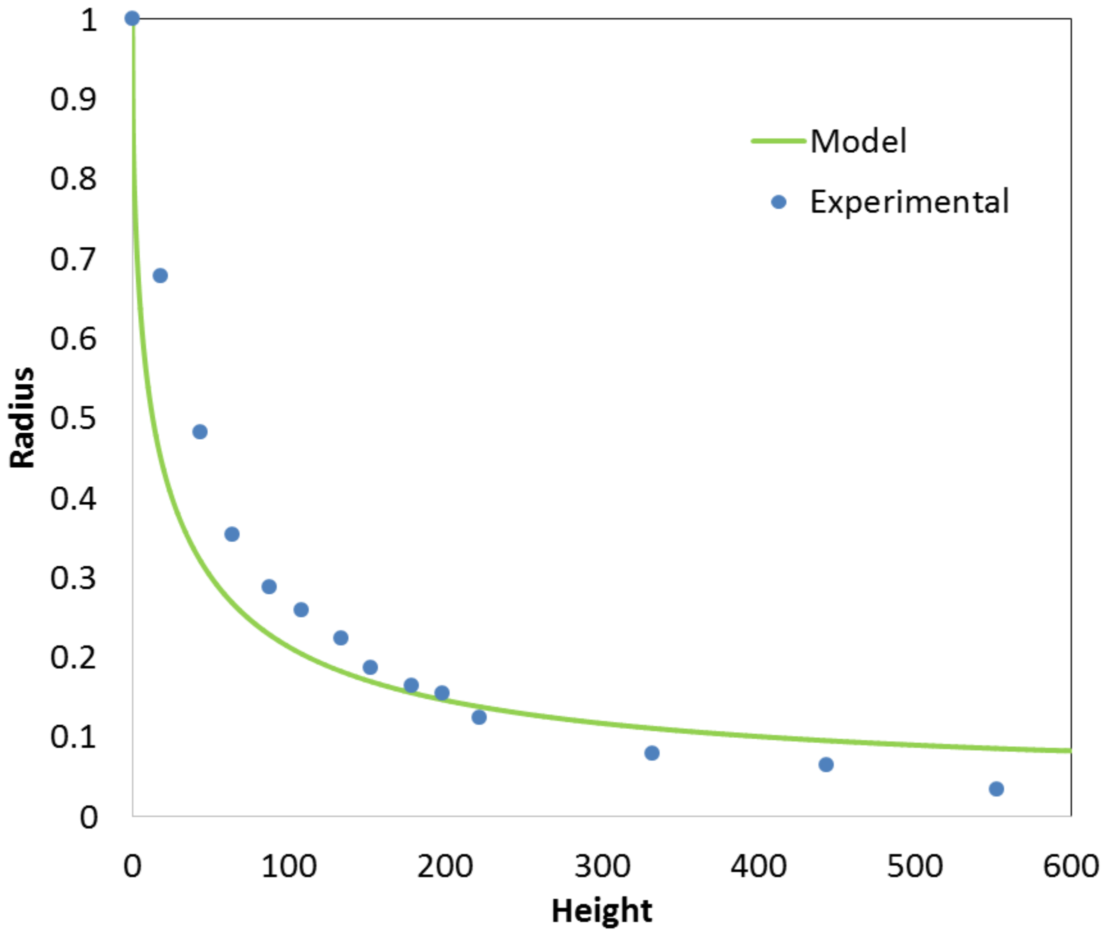
- C) All parameters as above with a higher conductivity $K=4.8*10^{-6}$ S/m, corresponding to Pe=$3.823*10^{-5}$, $\varepsilon=3.173*10^{-2}$, and E_∞=28.32.



Hohman et al, ''Electrospinning and electrically forced jets: II. Applications,'' Phys. Fluids **13**, 2221 (2001).

Giesekus model - Validation against Experimental Data

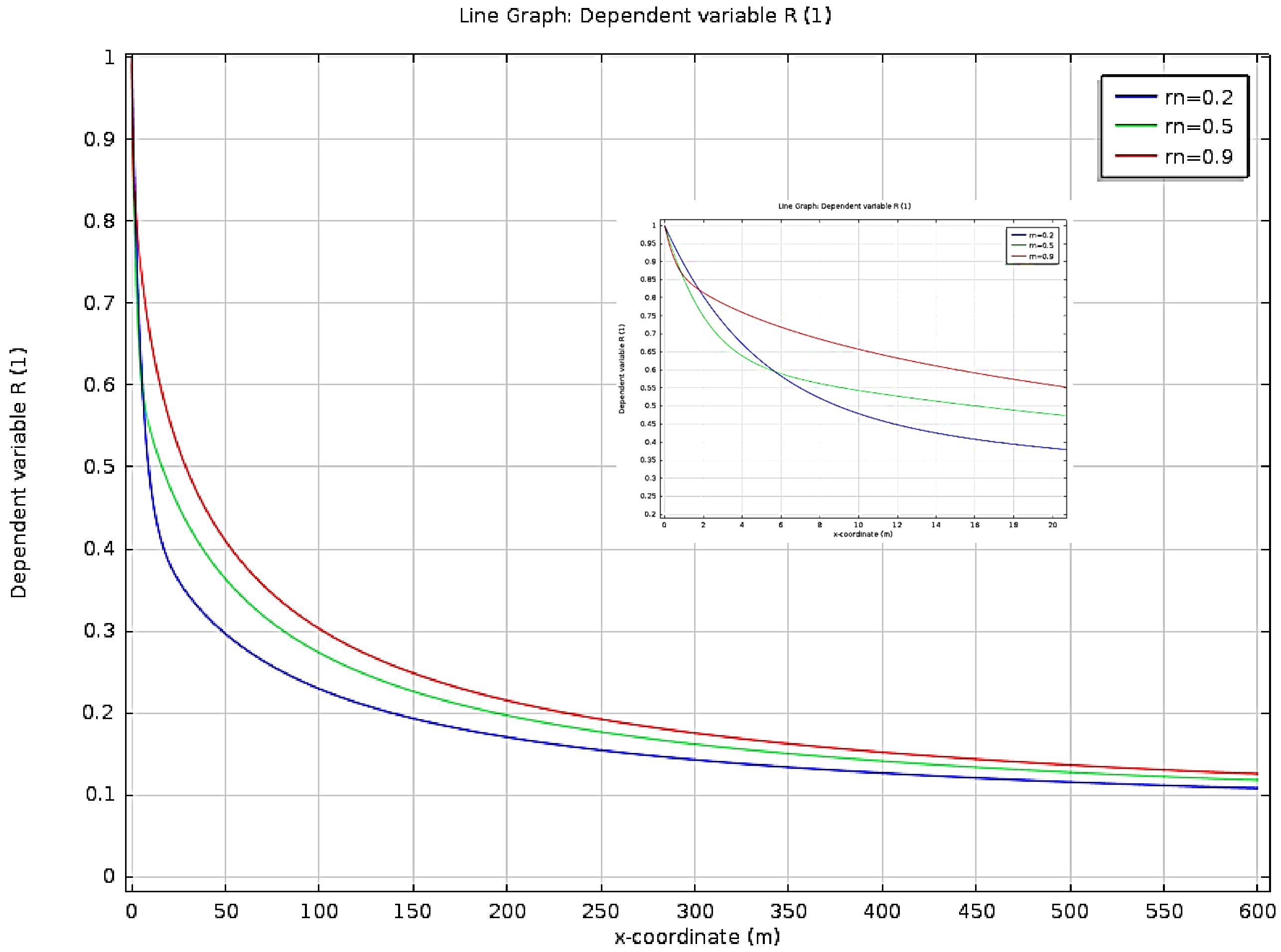
- Experimental data of Doshi et al. for a 4% PEO solution compared against our model.
- Electric field ($E\infty$ = 40 kVm−1)
- Nozzle radius ($R0$ = 45 m)
- length of the straight jet (L = 30 mm).
- The density ρ = 1.2 × 103 kgm−3
- dielectric constant, $\epsilon / \bar{\epsilon}$ = 42.7
- Viscosity, η_0 = 12.5 P;
- surface tension, γ = 76.6 dyn cm−1
- Conductivity, K = 4.902 × 10−3 Ω −1 m−1.
- The solvent viscosity is η_s = 10−2 poise for water
- I = 0.12 A
- Q = 10 μl min−1.



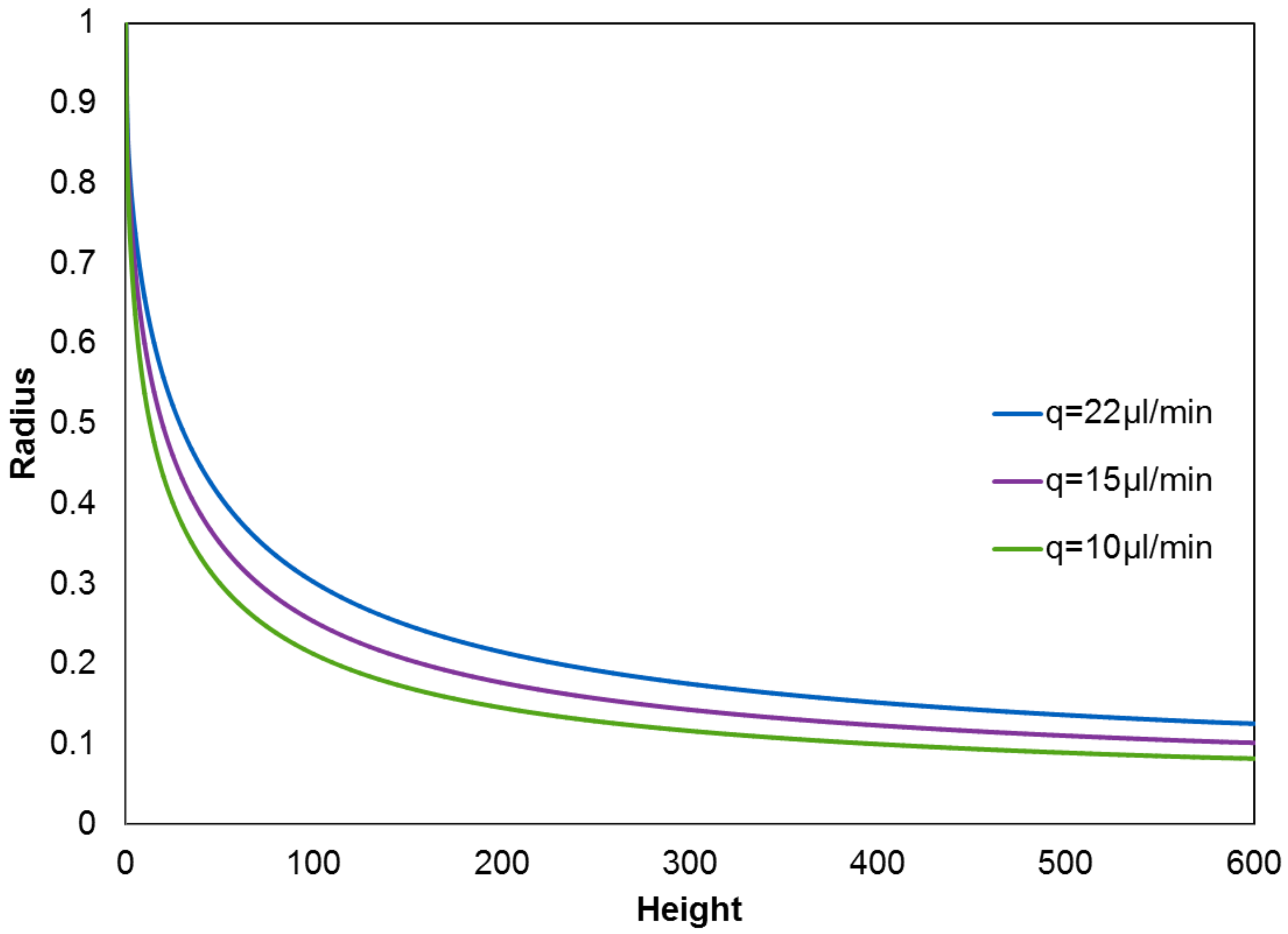
Doshi et al, Electrospinning and applications of electrospun fibers, J. Electrostat. 35 (1995) 151–160

Giesekus Model-Variation with viscosity ratio (r_η)

- Radius vs z



Giesekus Model-Variation with volumetric flow rate (Q)



Conclusion

- A mathematical model was built and validated against experimental data for Newtonian jet and Feng’s model for Non- Newtonian jets.
- The model was validated against experimental data for Giesekus model and extended to Oldroyd-B model.
- The model was extended for polymer solution with Non- Newtonian solvent.
- The dependence of the process on different working and material parameters was studied.

THANK YOU