Arc discharges under atmospheric pressure are often used for nanomaterial synthesis (e.g. boron nitride/carbon nanotubes or fullerenes). Feedstock for nanomaterial synthesis is produced by ablation of the arc electrodes, creating a jet that propagates from the inter-electrode gap into the ambient background gas [1]. Flow patterns in the jet were obtained analytically using boundary layer theory. Theoretical limits were verified via comparison to computational fluid dynamics (CFD) simulations. These simulations were based on a full set of Navier-Stokes equations and were, in turn, validated via comparison to experimental data [1]. For this research, the effects of boundary conditions, viscosity, and other variables on the flow pattern were studied both analytically and numerically. Additionally, the jet shape distortion caused by convection of the surrounding gas (heated by the electrodes) was studied.

[1] S. Yatom *et. al*, "Synthesis of nanoparticles in carbon arc: measurements and modeling", MRS. Comm. (2018), published online, doi:10.1557/mrc.2018.91.

Numerical Simulation of Arc Initiated Jet Flow

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Introduction

- A commonly used technique for creating nanomaterials (such as nanotubes or fullerenes) is to initiate an arc discharge under atmospheric pressures
- Ablation from the electrodes then creates a jet that flows out of the inter-electrode gap into the ambient gas, and in the process cools to form said nanomaterials, experimental data of which is shown below in Figure 1

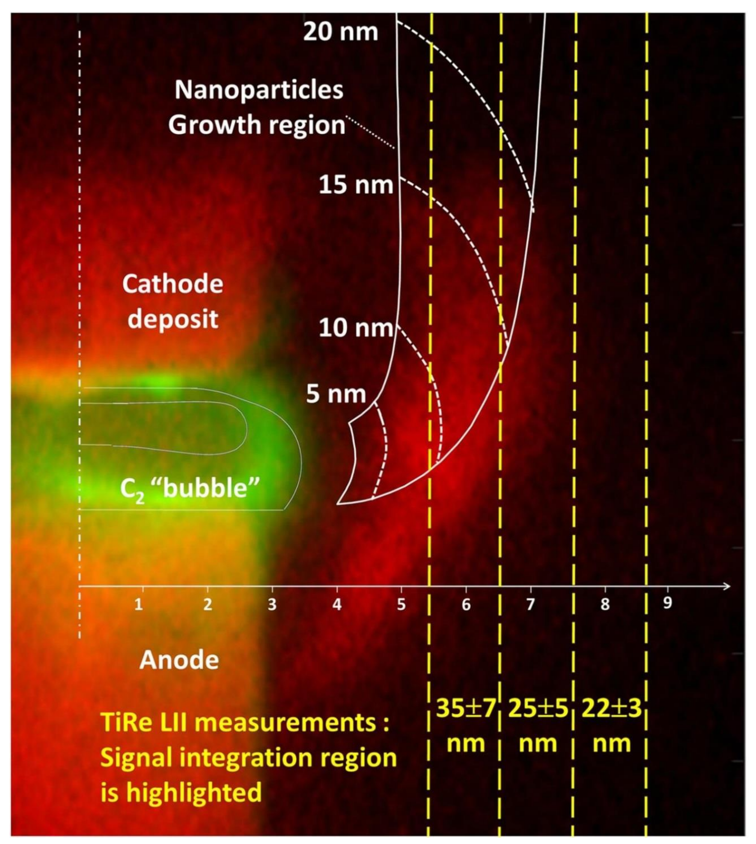

Figure 1: Experimental data [1] showing the arc region as well as the region where the majority of nanomaterial formation occurs. Note that this is experimental data, and therefore convection, outlet placement, and other factors break the top-bottom symmetry seen in other figures.

- In order to better predict the formation of nanomaterials, we investigated the flow patterns within the jet and compared them with a simple analytical solution

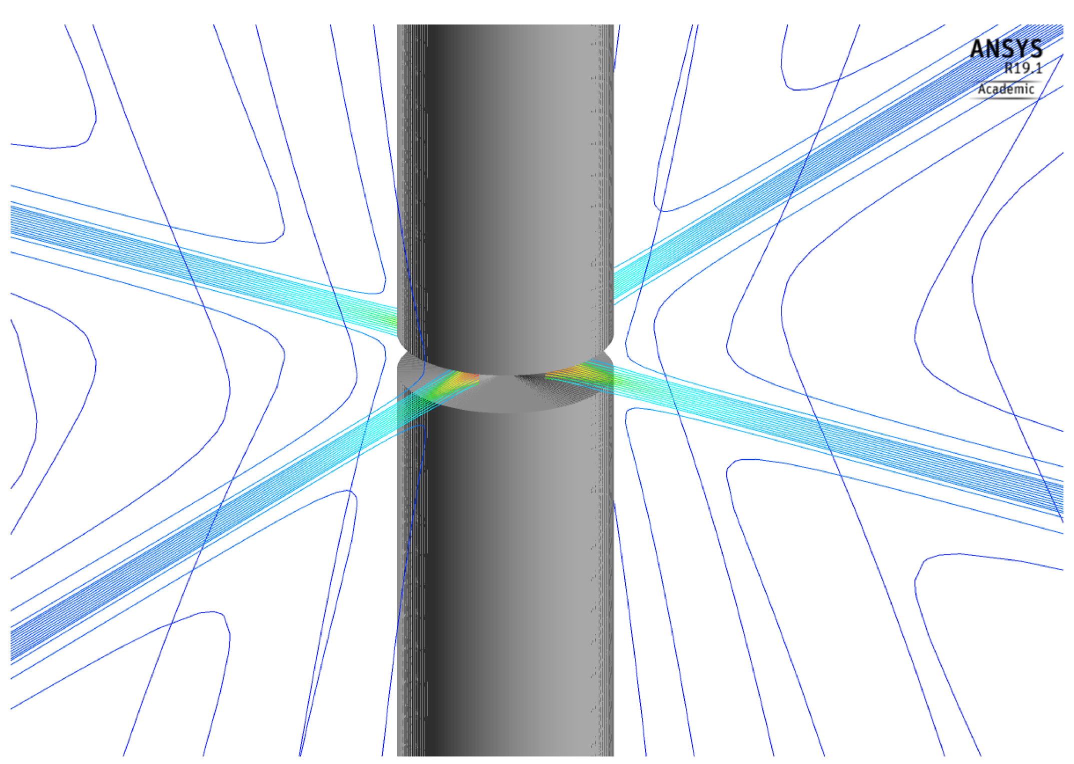

Figure 2: 3D diagram showing streamlines of the arc jet as well as streamlines of the ambient gas being entrained by the jet.

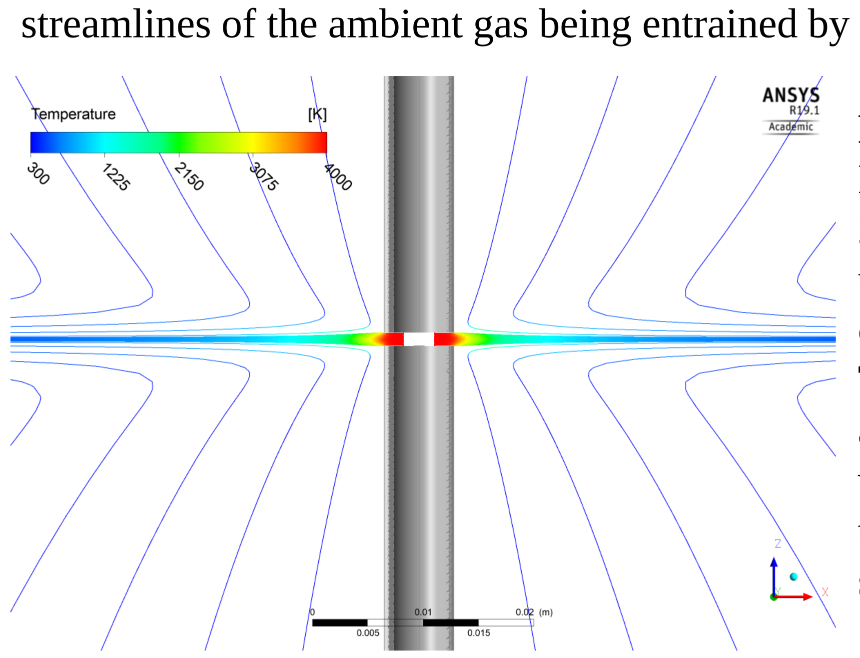

Figure 3: Diagram of the 2° sector actually used for computations. This is sufficient as axisymmetry was assumed in the analytical solution.

Analytical Solution

- Analytical solutions for flow patterns in the jet were derived via boundary layer theory assuming axisymmetric flow, following a procedure similar to that done by Schlichting [2]
- In order to keep these assumptions accurate, our flows were kept in the laminar regime, with low Mach numbers (≤ 0.06)
- Our solution can be formulated in terms of two different sets of independent variables (r, ψ, ν, Q_0, r_0) and (r, ψ, ν, ρ, J_0):

$$z = \sqrt[3]{\frac{16\,\rho\nu^2}{3\;J_0}}\, r \tanh^{-1}\left(\sqrt[3]{\frac{2}{3}\frac{\rho}{\nu J_0}}\,\frac{\psi}{r}\right) = \frac{4\nu r_0}{Q_0}\, r \tanh^{-1}\left(\frac{2r_0}{Q_0}\frac{\psi}{r}\right)$$

- Where "ρ" is the (constant) density of the gas, "ν" is the dynamic viscosity, "J_0" is the initial (at the outlet) momentum flow rate, "ψ" is the stream function, "r_0" is the radius of the electrodes, and "Q_0" is the initial volumetric flow rate
- In order to compare our solution against those made previously, we used as a baseline the equations derived by Hunt & Ingham [3]

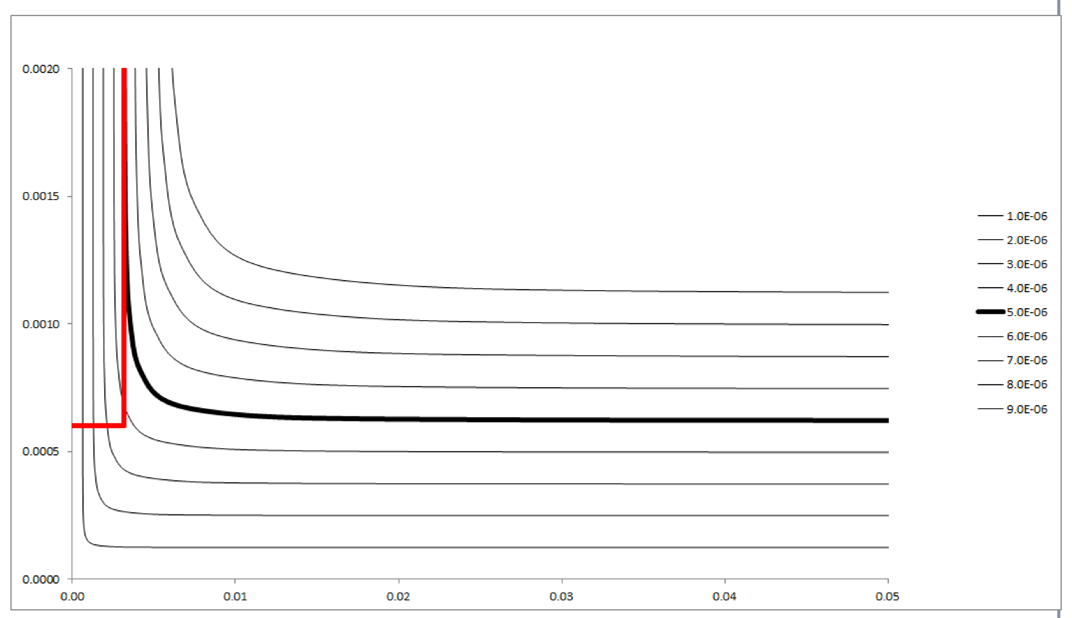

Figure 4: A sample analytic solution for the streamlines along and inside the jet. Note that the top electrode here is outlined in red, and that the centerline of the jet lies on the line y=0

Simulations & Results

- In order to check the verify the analytical solutions, numerical simulations were performed using ANSYS CFX, which is based on a full set of Navier-Stokes equations
- Numerous different variables, meshes, and boundary conditions were tested as shown in Figures 5-10 below

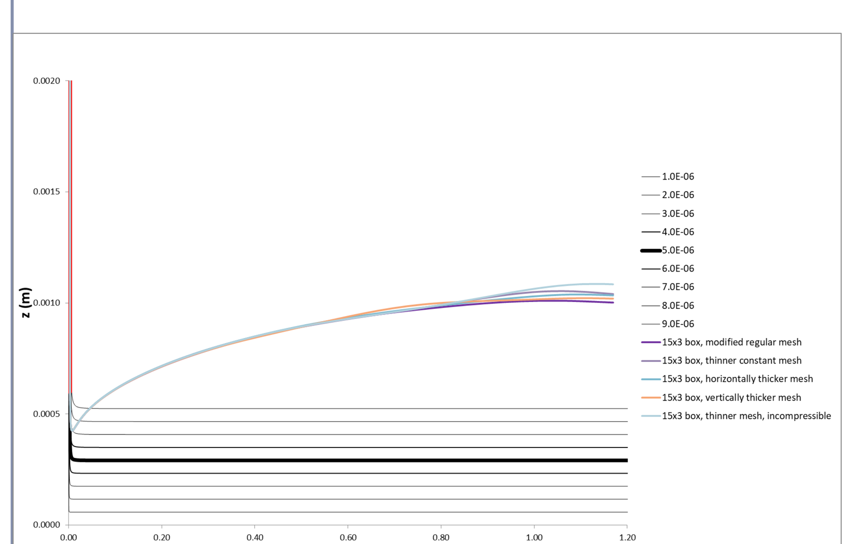

Figure 5: Plot of the computational streamlines obtained with different boundary conditions and meshes.

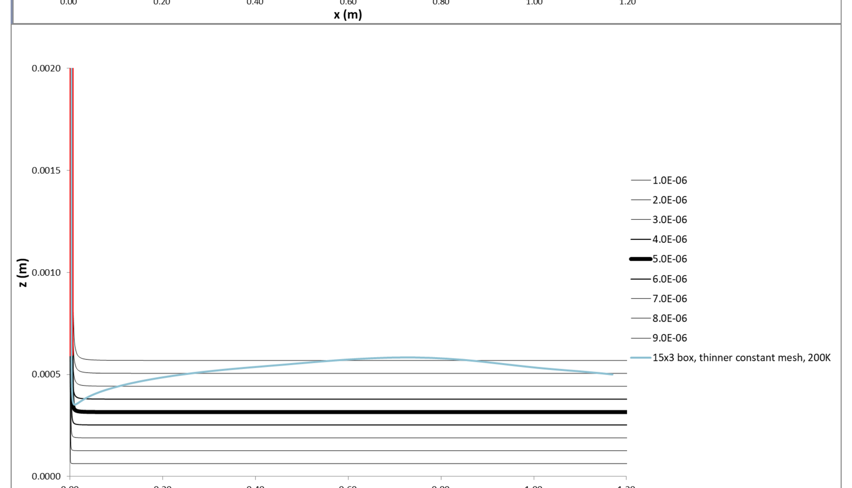

Figure 6: Plot of the computational streamline obtained for an ambient air temperature of 200K. Note that it falls much closer to the analytical solution than the 300K plots of Figure 5.

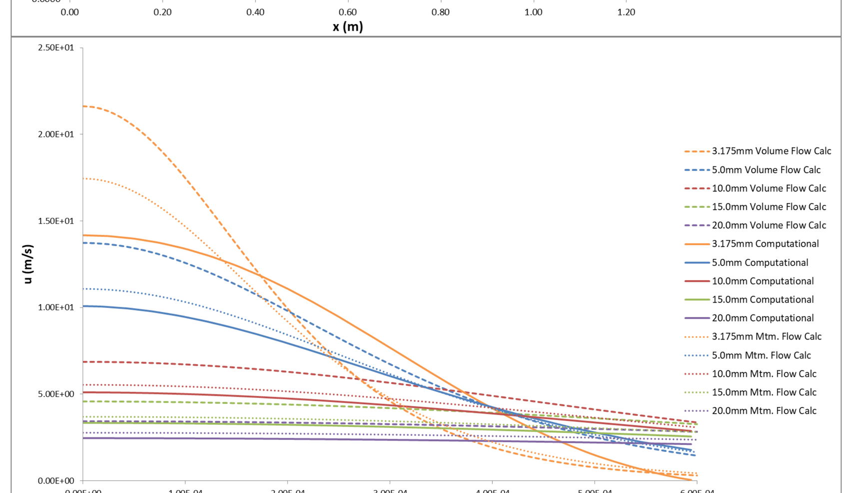

Figure 7: Plot of the analytical and computational velocity distributions across the jet at varying x positions.

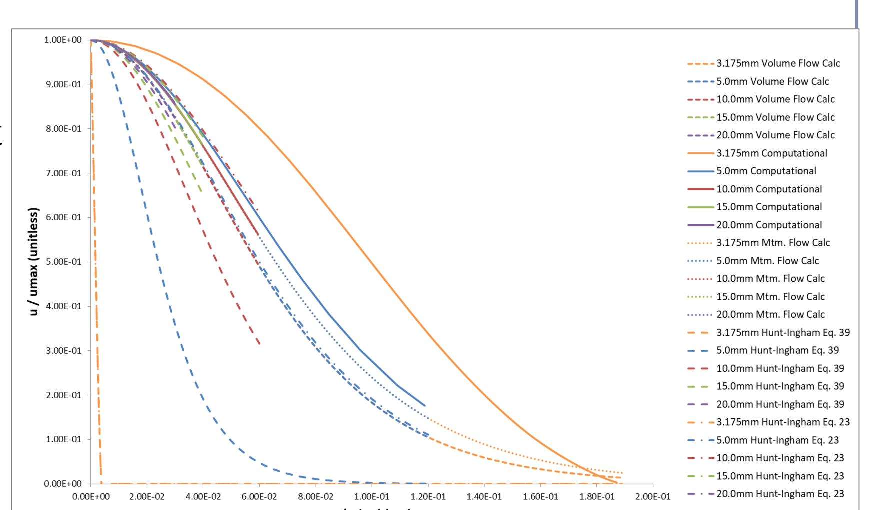

Figure 8: The same data as Figure 7, but now scaled on both axes, and plotted with the two Hunt-Ingham analytical equations.

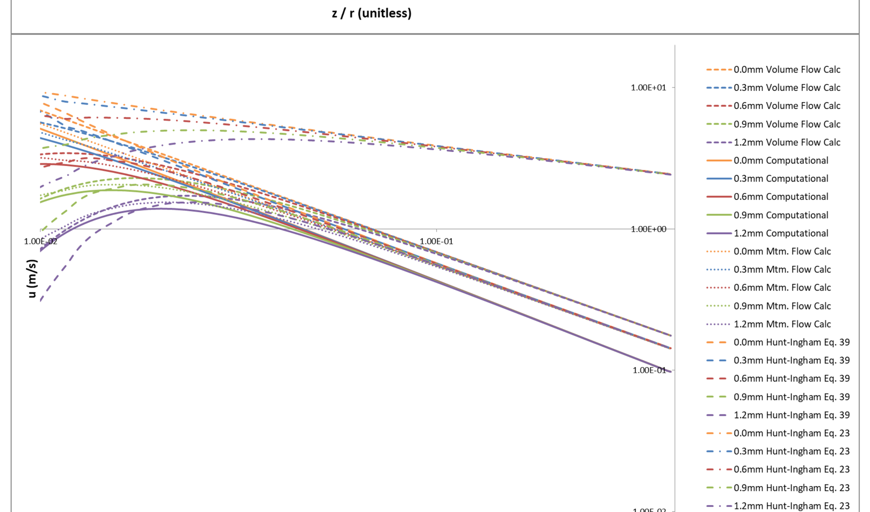

Figure 9: Plot of the analytical and computational velocity distributions along the jet at varying z positions. (Note this is a log-log plot).

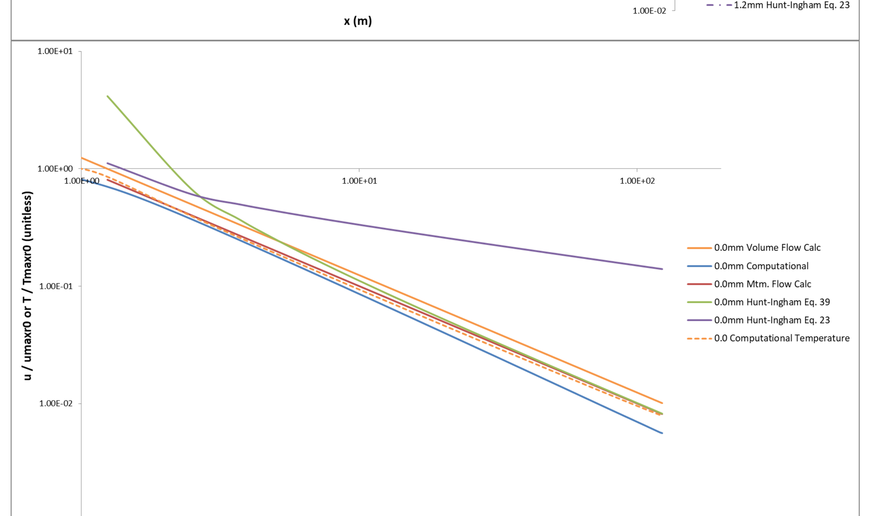

Figure 10: The data from z=0 of Figure 9, but now scaled on both axes, and plotted with the computational temperature distribution along the jet (Note this is a log-log plot).

Conclusions

- As seen in Figure 5, our results appear to be fairly independent from the type of boundary condition or thickness of mesh used
- In general, our analytical solution obtains greater accuracy with lower temperatures, smaller gap sizes, and at distances further from the gap
- As seen in Figures 8-10, our momentum flow analytical solution fits better with the computational data than the Hunt-Ingham equations, even at areas close to the gap
- However, our momentum flow solution remains off from the computational values by a multiplicative factor; this, presumably, is due to viscous effects not accounted for by boundary layer theory
- We are also able to predict the temperature distribution along the jet, as seen in Figure 10

Future Work

- In the future, one could take into account more complex physical factors, such as convection, outlet placement, and carbon deposition
- More complex computational results should also be verified by experiment
- Additionally, one could correct for the viscous effects of the jet and thus find better agreement between the analytical and computational solutions

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[1] S. Yatom et. al, "Synthesis of nanoparticles in carbon arc: measurements and modeling", MRS. Comm. (2018), published online, doi:10.1557/mrc.2018.91.

[2] Schlichting H, Gersten K (2017) Boundary-layer theory. Springer, Berlin

[3] Hunt, G.R. & Ingham, D.B. Acta Mechanica (1998) 127: 25. https://doi.org/10.1007/BF01170360

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