# Accelerating Design Exploration and Optimization with Surrogate Physics Models

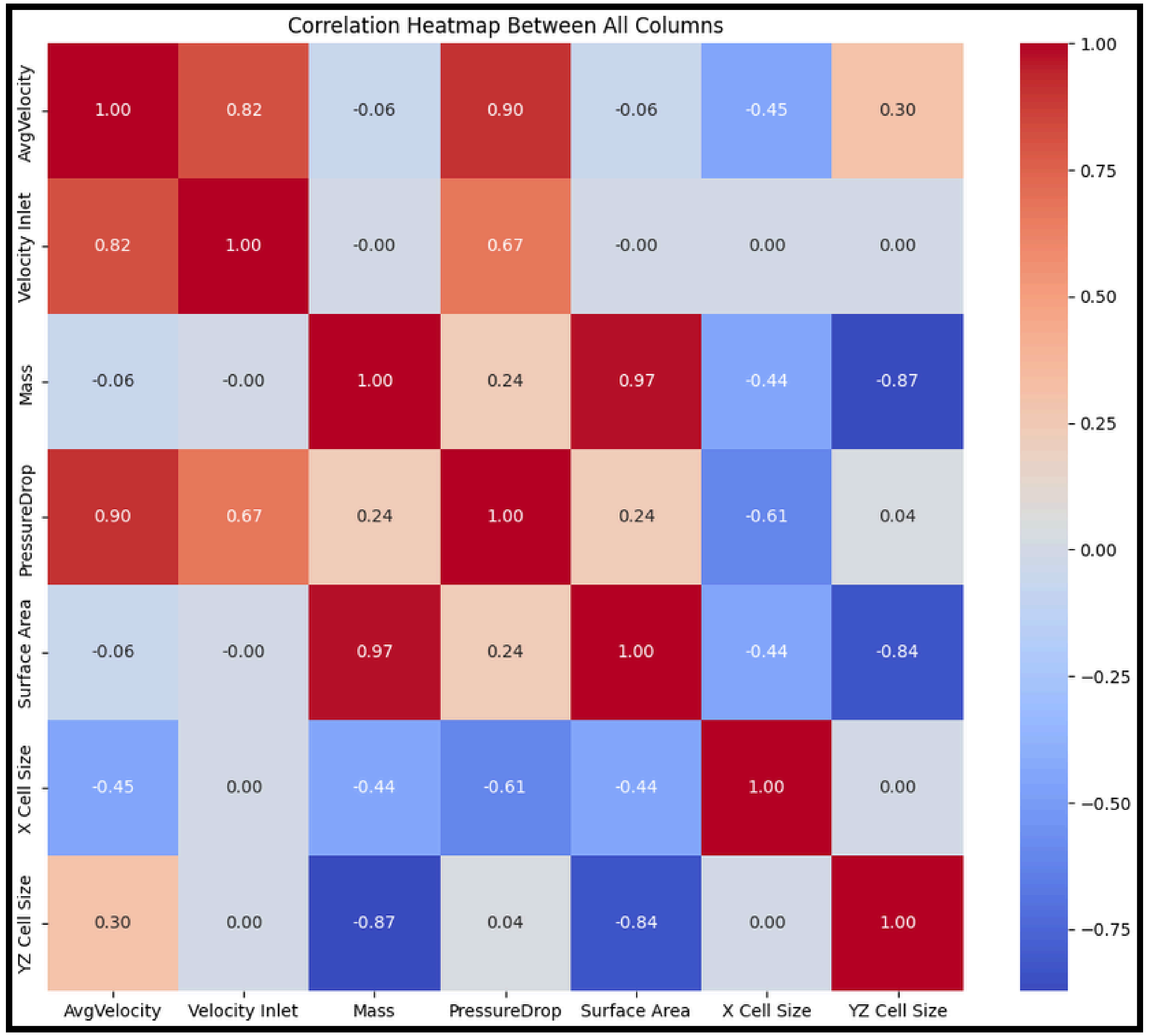
Presented by Rishabh Jain & Shiv Ratn
IIT Delhi

# Dataset

## Input:
- Cell Size X
- Cell Size YZ
- Average Velocity

## Output:
- Mass
- Surface area
- Average Velocity
- Pressure Drop

Inference:
- There is absolutely no correlation between Mass and Inlet Velocity
- There is absolutely no correlation between Surface Area and Inlet Velocity



# Involved Physics

Mass:

- Smaller cell size → Higher Mass

Surface Area:

- Smaller cell size → Higher Surface Area

- Flow Volume = $V_s$
- Pressure Drop = $\Delta p$
- Inlet Velocity = $v$
- Submerged Area = $A_s$
- Hydraulic diameter: $D_h = 4V_s/A_s$
- Reynolds number: $Re = \rho D_h v/\mu$

Note : $D_h$ = f(Mass, Surface Area)

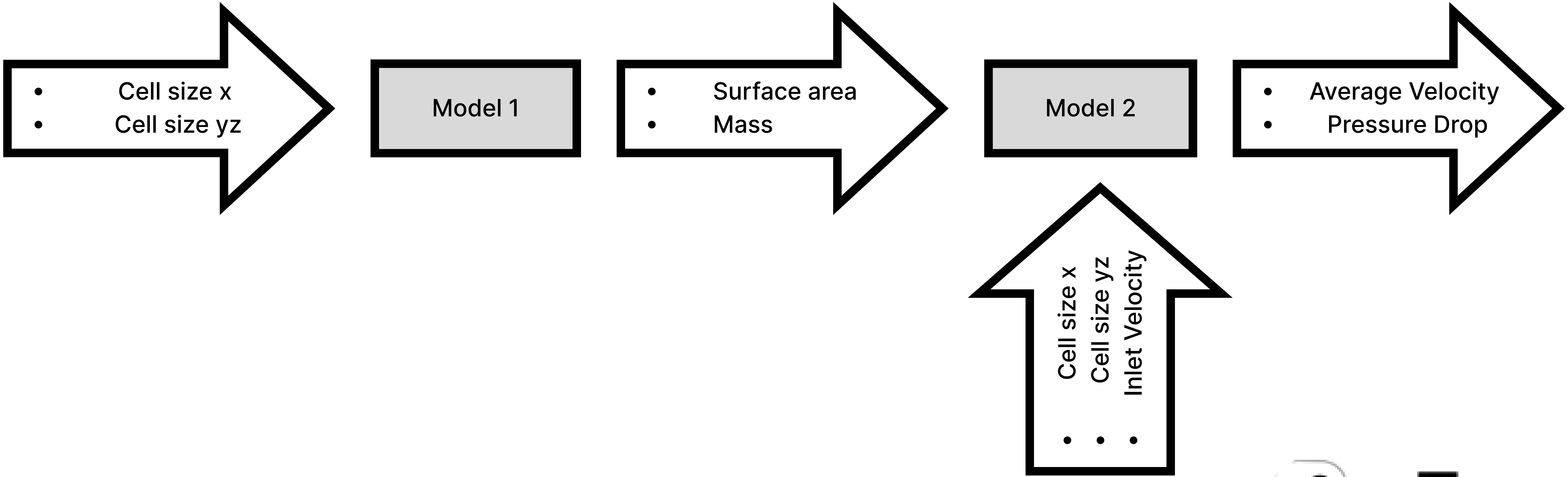
Average Velocity:

- Avg. velocity scales with **Inlet Velocity**
- smaller **Dh** → higher flow resistance
- **Cell Sizes** determine Directional Anisotropy

Pressure Drop:

- Pressure drop : $\boldsymbol{\Delta p \propto v^2/D_h}$
- Flow Volume is governed by **Mass**
- **Cell Sizes** determine Directional Anisotropy

# Surrogate Model Architecture



# Model Specifications

Model 1 :
Number of layers = 3
Neuron Count = [237, 182, 240]
Activation Function = Leaky ReLU
Optimizer = Adam
Learning Rate = 0.006745
Batch Size = Full Batch

Model 2 :
Number of layers = 3
Neuron Count =[262, 469, 70]
Activation Function = ReLU
Optimizer = Adam
Learning Rate = 0.002447
Batch Size = 32
Weight Decay = 2.939e-5

We used probabilistic approach to sample the best hyperparameters, likely to increase model accuracy

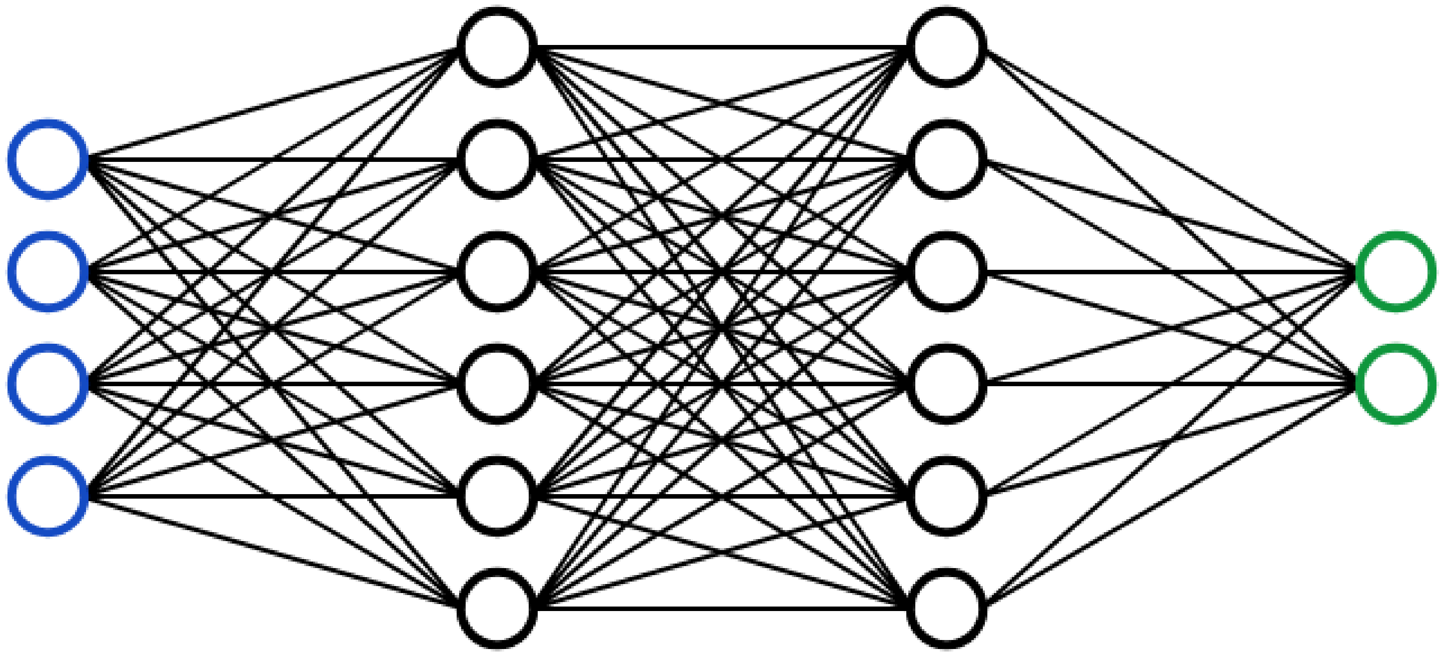


*Image source : https://victorzhou.com/series/neural-networks-from-scratch/*

# Optimization Algorithm

To find: Maximum Surface Area
Constraint:

- 10mm < Cell Size X < 25mm
- 10mm < Cell Size Y/Z < 25mm
- 2500 mm/s < Inlet Velocity < 3500 mm/s
- Mass < 125 grams
- Pressure Drop < 8000 Pa
- Avg Velocity > 520 mm/s^2

Initial Approach : Grid Search on Surrogate Model Function

- Form high resolution grid on the surrogate function
- Mask the grid points which satisfy the constraint
- Choose the highest surface area from the set of masked grid points

**Optimization output :** Cell Size X = 15.2968 ; Cell Size YZ = 24.9843 ; Inlet Velocity = 2585.78 ; Surface Area = 23689.015 ; Mass = 124.99 ; Pressure Drop = 5859.8662 ; Average Velocity = 541.834

Average Velocity and Pressure Drop is not the “limiting constraint”

↓

We only optimize the Surface Area with the Mass constraint
(Optimization limited to Model 1)

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# Simplified Optimization Problem

Constraints on Inlet Velocity, Pressure Drop and Average Velocity are NOT A LIMITING CONDITION

### Stage 1 — Cell Size Optimization

- **Objective:** maximize surface area (implemented as minimizing −surface_area)
- **Constraint:** mass < 125 g (enforced via heavy penalty: penalty = (mass − 125) * 10000 when violated)
- **Algorithm:** global search with Differential Evolution (seeded) + multi-start local refinement with L-BFGS-B
- **Output:** optimal_x, optimal_yz, predicted mass & surface area

### Stage 2 — Inlet velocity feasibility

- **Sweep inlet velocity** ∈ [2500, 3500] mm/s (grid)
- Use Model2 to predict AvgVelocity and PressureDrop
- Feasibility criteria:
- AvgVelocity > 520 $mm/s^2$
- PressureDrop < 8000 Pa
- Output: feasible velocity range, recommended solution (middle of feasible range)

### How the code uses Diffenrential Evolution + local polish

- DE finds promising basins (global exploration).
- TwoStageOptimizer then runs multi-start L-BFGS-B (20 random starts in the notebook) to quickly refine to a precise local optimum inside those basins.
- This combination gives robust global coverage (DE) plus fast accurate convergence (L-BFGS-B).

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# Results

Optimization output :

Cell Size X = 21.787

Cell Size YZ = 20.5293

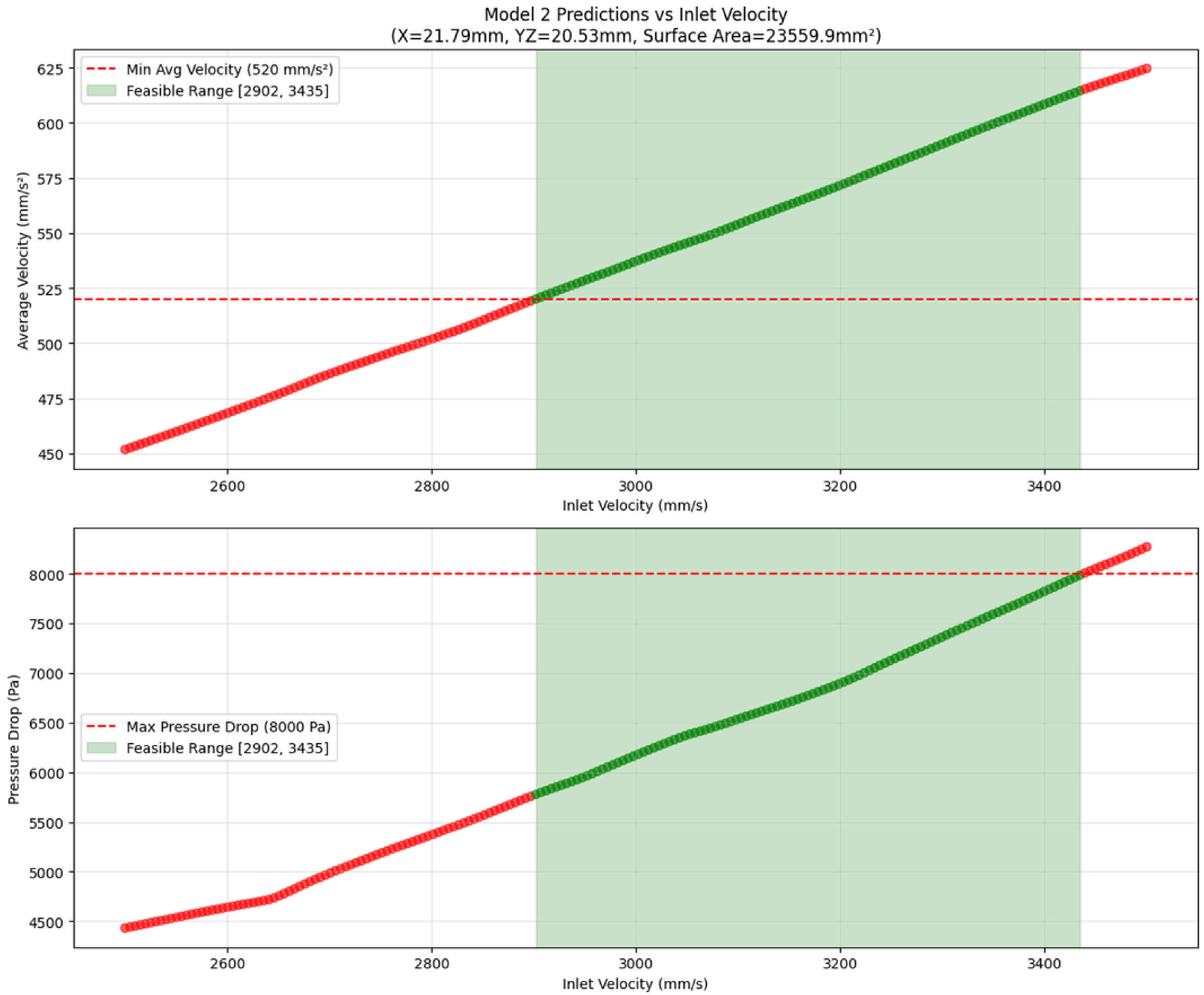
Inlet Velocity = 3168.3

Surface Area = 23559.94

Mass = 124.99

Pressure Drop = 6772.29

Average Velocity = 566.02



# Thankyou