Predicting Complex Erosion Profiles in Steam Distribution Headers with Convolutional and Recurrent Neural Networks

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Outline

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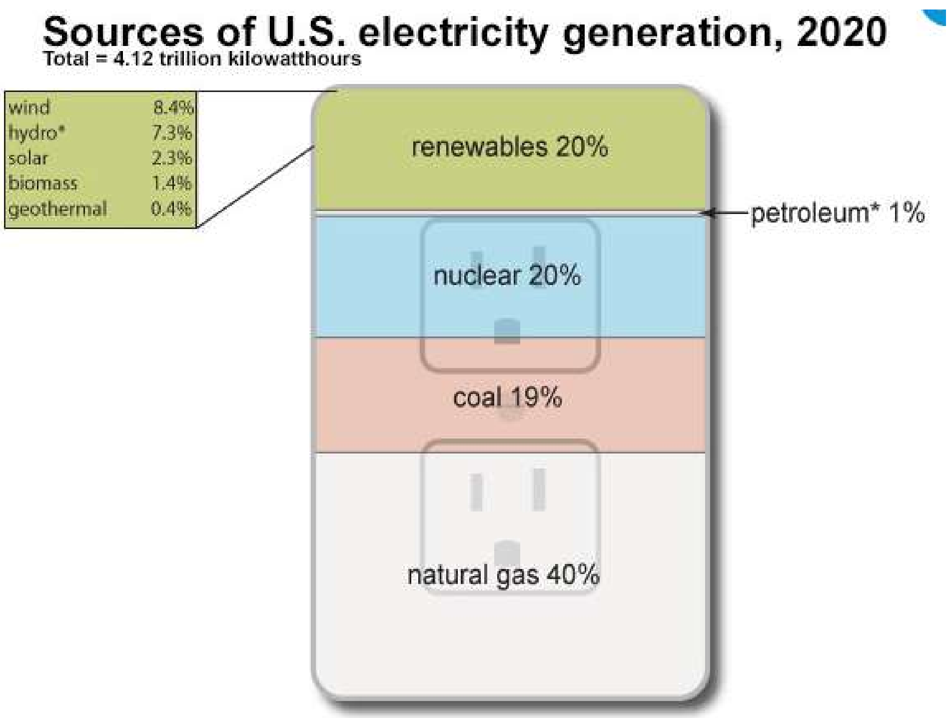
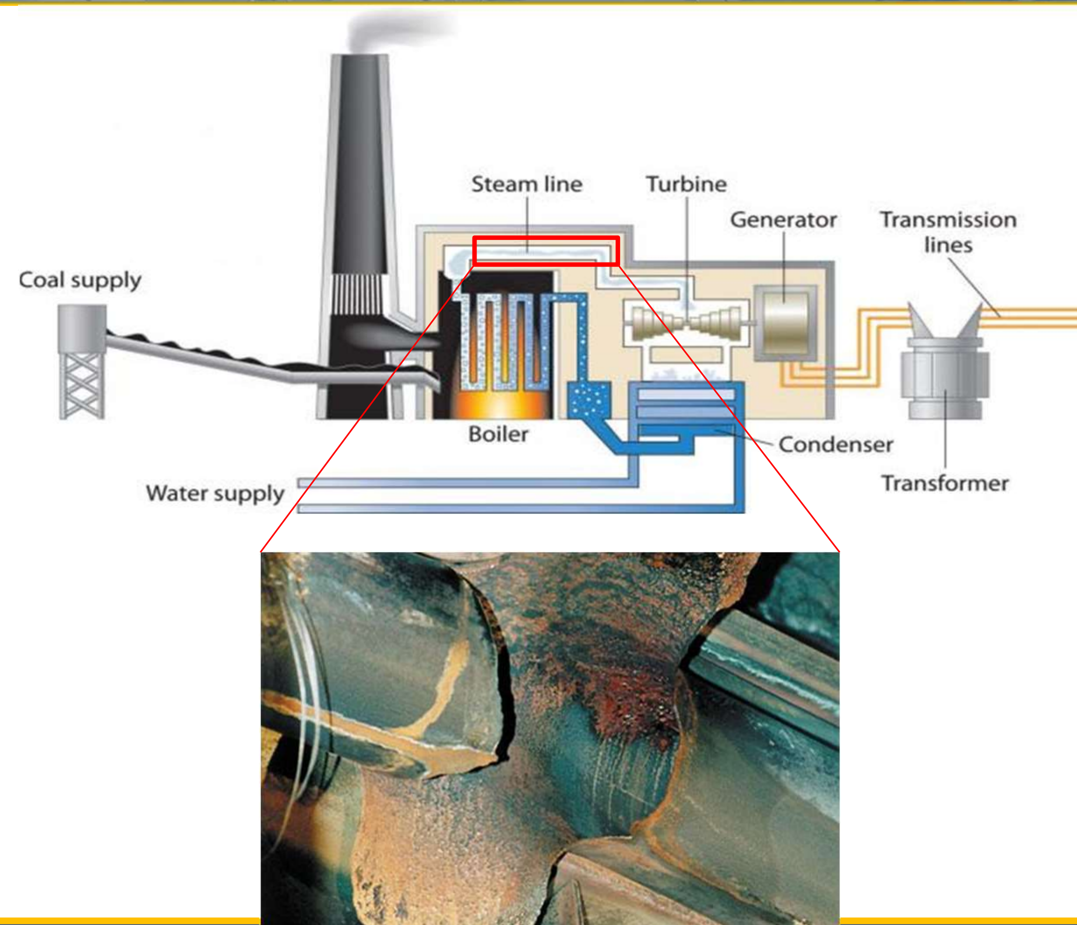
   a) Background
   b) Computational Fluid Dynamics (CFD) with ANSYS Fluent
   c) Case study on Steam Distribution Header Module OP-650
   d) ML Approach – Long Short-Term Memory (LSTM) Recurrent Neural Network + Convolutional Neural Network (CNN)

2. Result and Discussion
   a) Results
   b) Feature Importance Analysis
   c) Computational Time Comparison

3. Conclusion

U.S. Electricity Generation with Coal





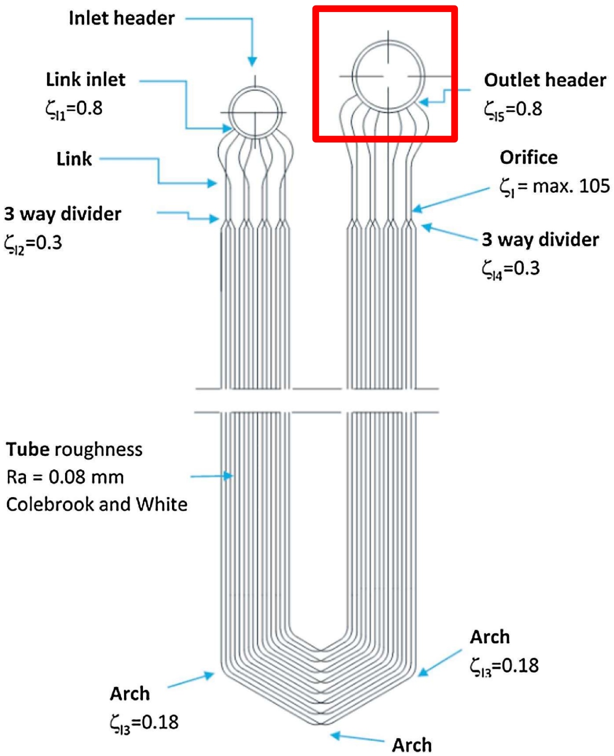
U.S Energy information administration

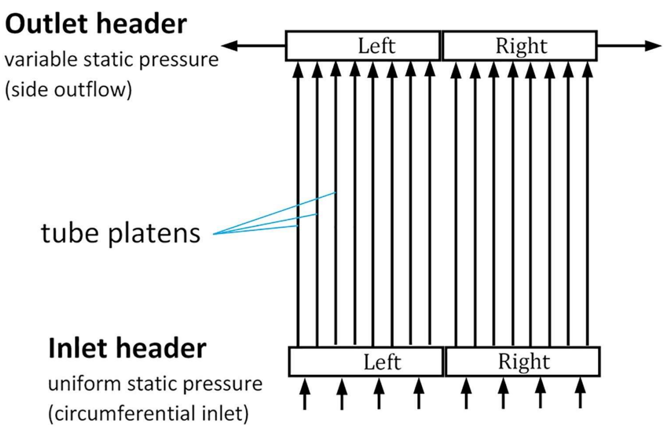
Computational Fluid Dynamics (CFD)

- **Computational fluid dynamics (CFD)** simulates erosion from particle impingement. It replaces **Reynolds-Averaged Navier Stokes equation** with algebraic difference equations to solve fluid flow problems.

Advantages	Disadvantages
Simulations contribute to greater understanding of problem	Complex task involving various phenomena that must be considered
Costs usually much lower compared to experiments	Computation time may extend for large models
	Errors may occur due to simple flow models or simplified boundary conditions

Case study model - OP-650 steam distribution header





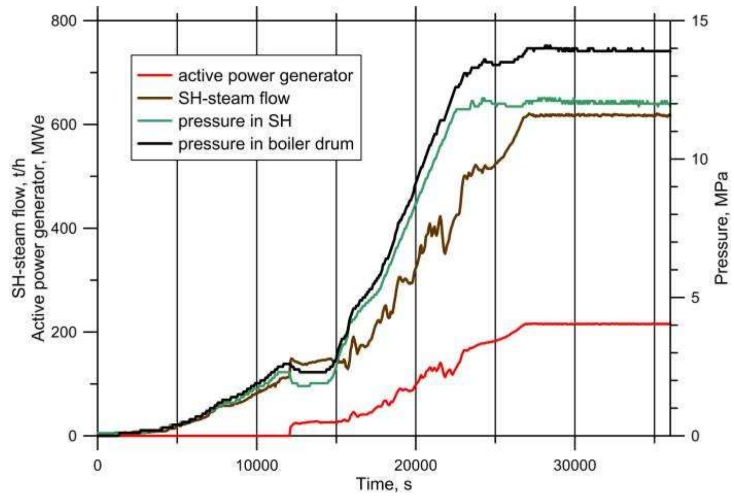
Diameter/tube thickness:

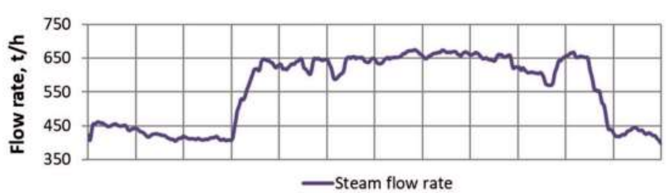
ϕ57/5 – link
ϕ44.5/4 – tube
ϕ406/14 – inlet header
ϕ558/30 – outer header

- In Poland, OP-650 boiler model is general design for sub-critical coal plant.
- A part of OP-650 steam distribution header was selected for geometric model for erosion prediction.

Modliński, Norbert, et al. "Mathematical procedure for predicting tube metal temperature in the second stage reheater of the operating flexibly steam boiler." Applied Thermal Engineering 146 (2019): 854-865.

Operating Parameter Range of OP-650





- Operating pressures determined from reference papers

Initial inlet speed range calculated from flow rate

$$v = \frac{f}{A}$$

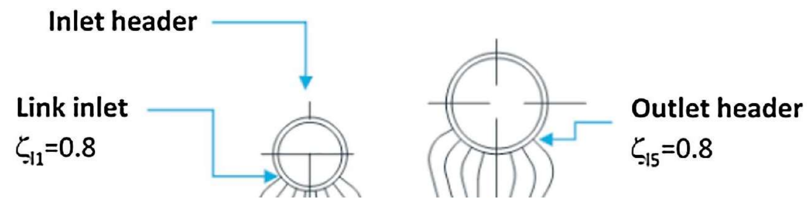
v = Steam velocity (m/s)
f = Flow rate(m^3/s)
A = Cross sectional area of pipe (m^2/s)

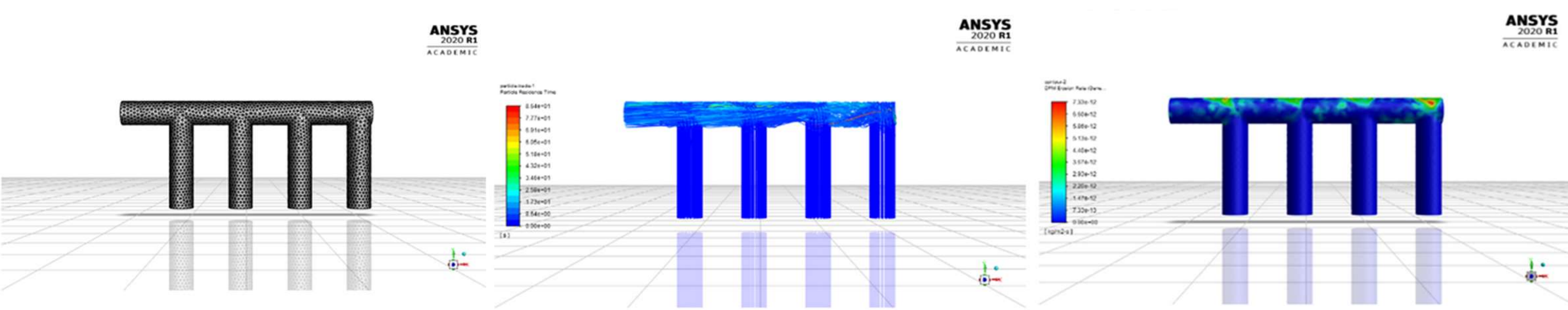
	Min	Max
Initial main-inlet speed (m/s)	16.75	27.12
initial sub-inlet speed (m/s)	237.03	430.06
Initial main-inlet pressure (MPa)	14	16
Initial sub-inlet pressure (MPa)	2.3	3.0

Modliński, N.; Szczepanek, K.; Nabagło, D.; Madejski, P.; Modliński, Z. Mathematical Procedure for Predicting Tube Metal Temperature in the Second Stage Reheater of the Operatin
Flexibly Steam Boiler. *Applied Thermal Engineering* **2019**, *146*, 854-865.

CFD-Based Erosion Modeling

- Used ANSYS Fluent v19.2 to generate data
- ANSYS automated meshing used to discretize domain

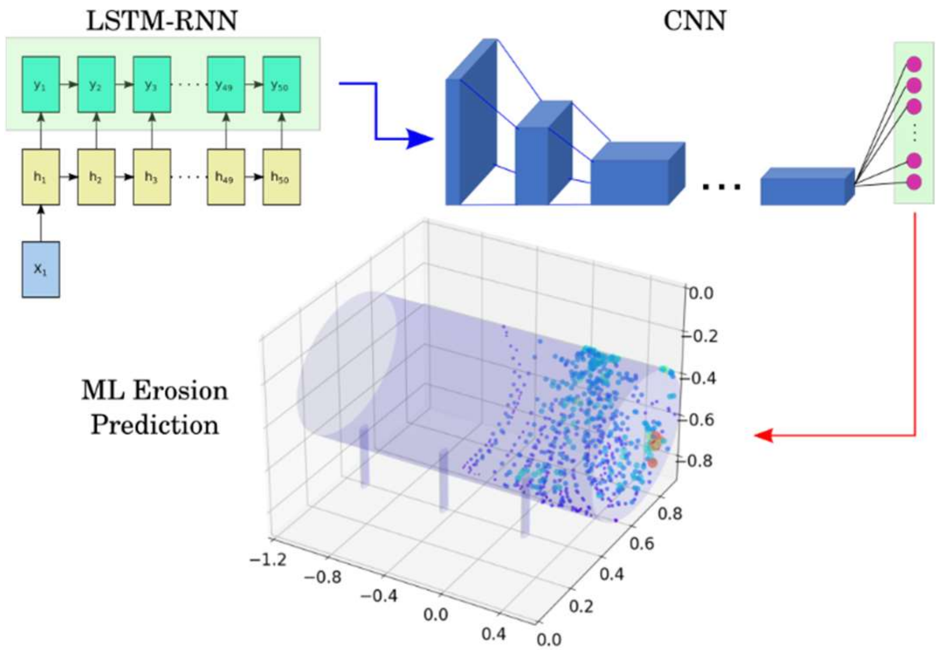




Mesh grid interface → Fluid flow modeling → Erosion modeling

Research Outline

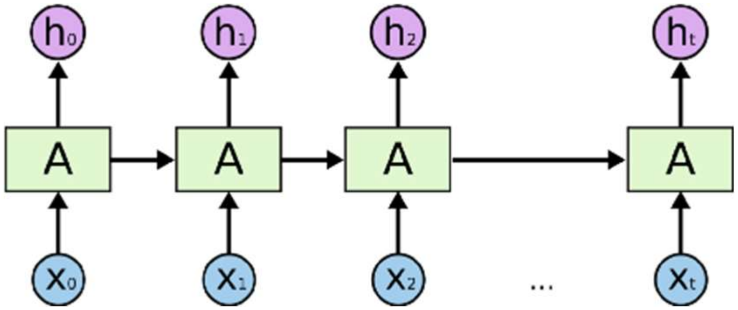
- Use Convolutional Neural Network (CNN) & Long and Short-Term Memory (LSTM) machine learning approaches to predict complex surface erosion profiles in steam distribution headers
  - Given only:
    (1) Particle size
    (2) Main-inlet speed
    (3) Sub-inlet speed
    (4) Main-inlet pressure
    (5) Sub-inlet pressure



Recurrent Neural Network (RNN)

- Recurrent Neural Networks (RNNs) are type of neural network that specialize in processing **sequences**
- RNNs allow **variable-length sequences** as both inputs & outputs.

- Long-term information sequentially travels through all cells before getting to present processing cell.
- Easily corrupted by being multiplied many times by small numbers – Vanishing gradient problem

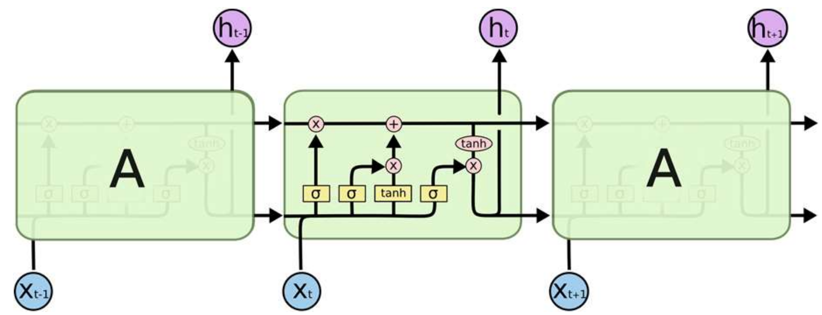


Sequential processing in conventional RNN

Long Short-Term Memory (LSTM)

- Long Short-Term Memory (LSTM) is special kind of RNN, capable of learning long-term dependencies.

- LSTM layers have multiple switch gates (additive & forget gates with 'tanh' activation function)
- **No vanishing gradient problem.** Can bypass units & remember for longer time steps.

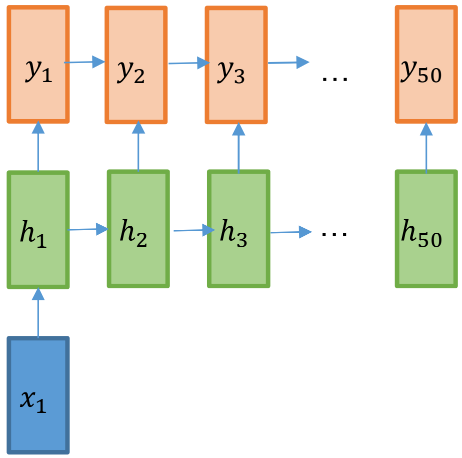


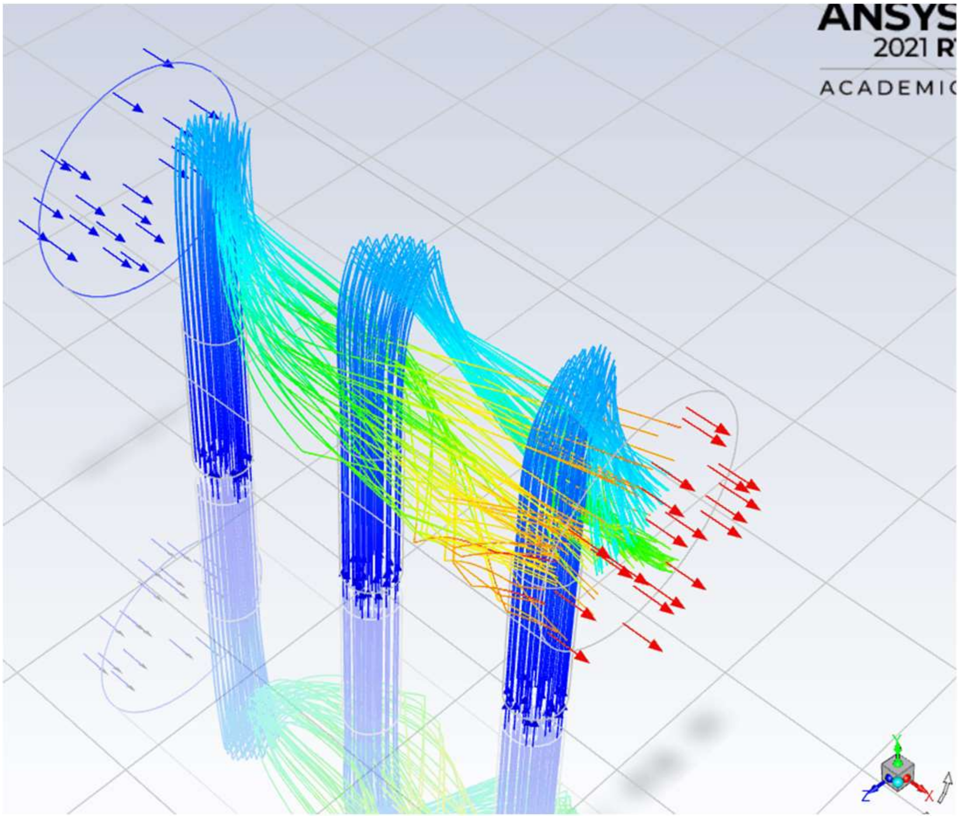
Sequential processing in LSTM

Colah.github

LSTM: Particle Trajectory Prediction

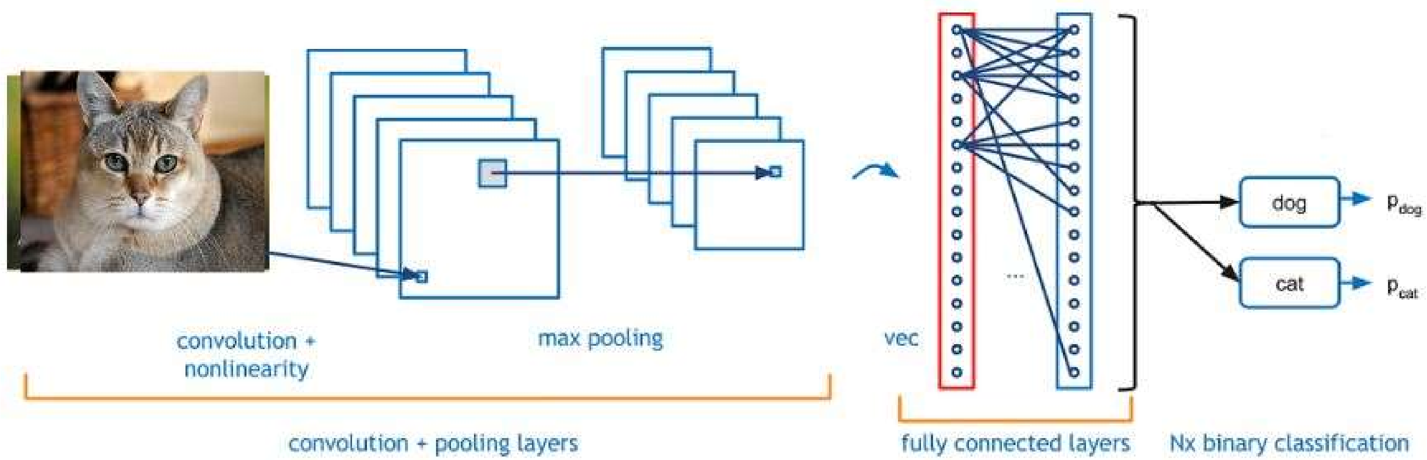
Hypothesis: Whole particle trajectory predictable with LSTM based on initial conditions such as initial positions, speeds, pressures, & particle sizes.





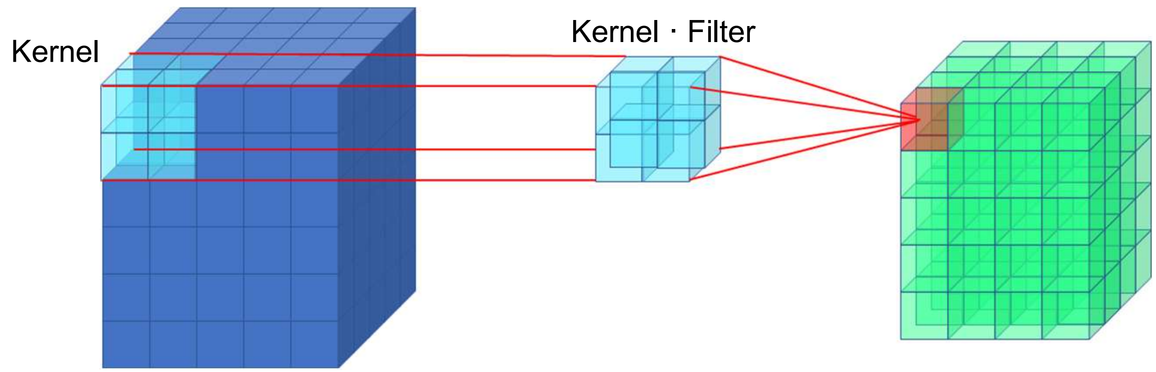
Convolutional Neural Network (CNN)

- CNN (convolutional neural network or ConvNet): class of deep neural networks, typically applied to analyze visual imagery by summarizing presence of features in input data.

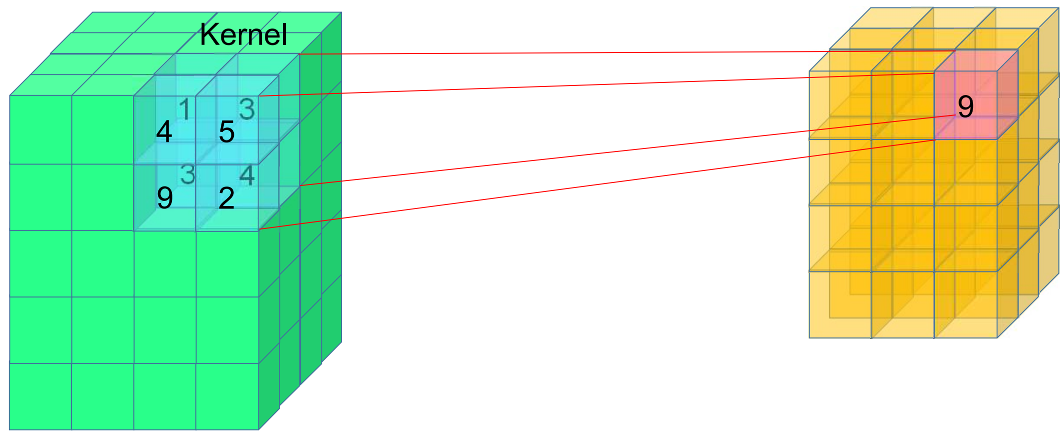


How CNN Works?

3D-Convolution: kernel values are multiplied with filter's values, then summed via **dot product** between kernel and the filter. The (2×2×2) kernel slides over by one voxel, repeating the process until kernel covers entire original data.



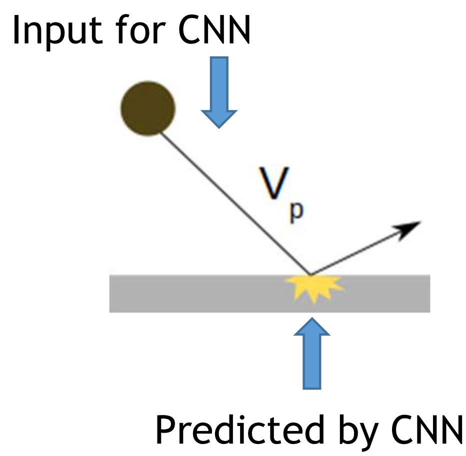
3D-Maxpooling: After convolution, maximum value in kernel is saved in output; kernel then strides by one voxel & repeats same operation.

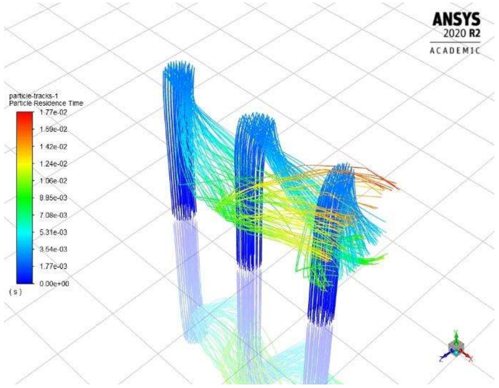


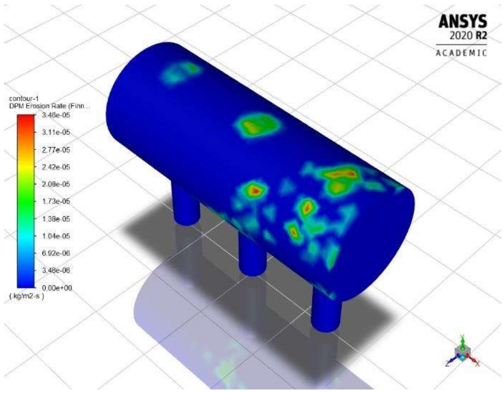
CNN: Erosion Rate Profile Prediction

Hypothesis: Erosion rate profile on geometry predictable when CNN model can identify & magnify features of erosion from particle trajectory data.

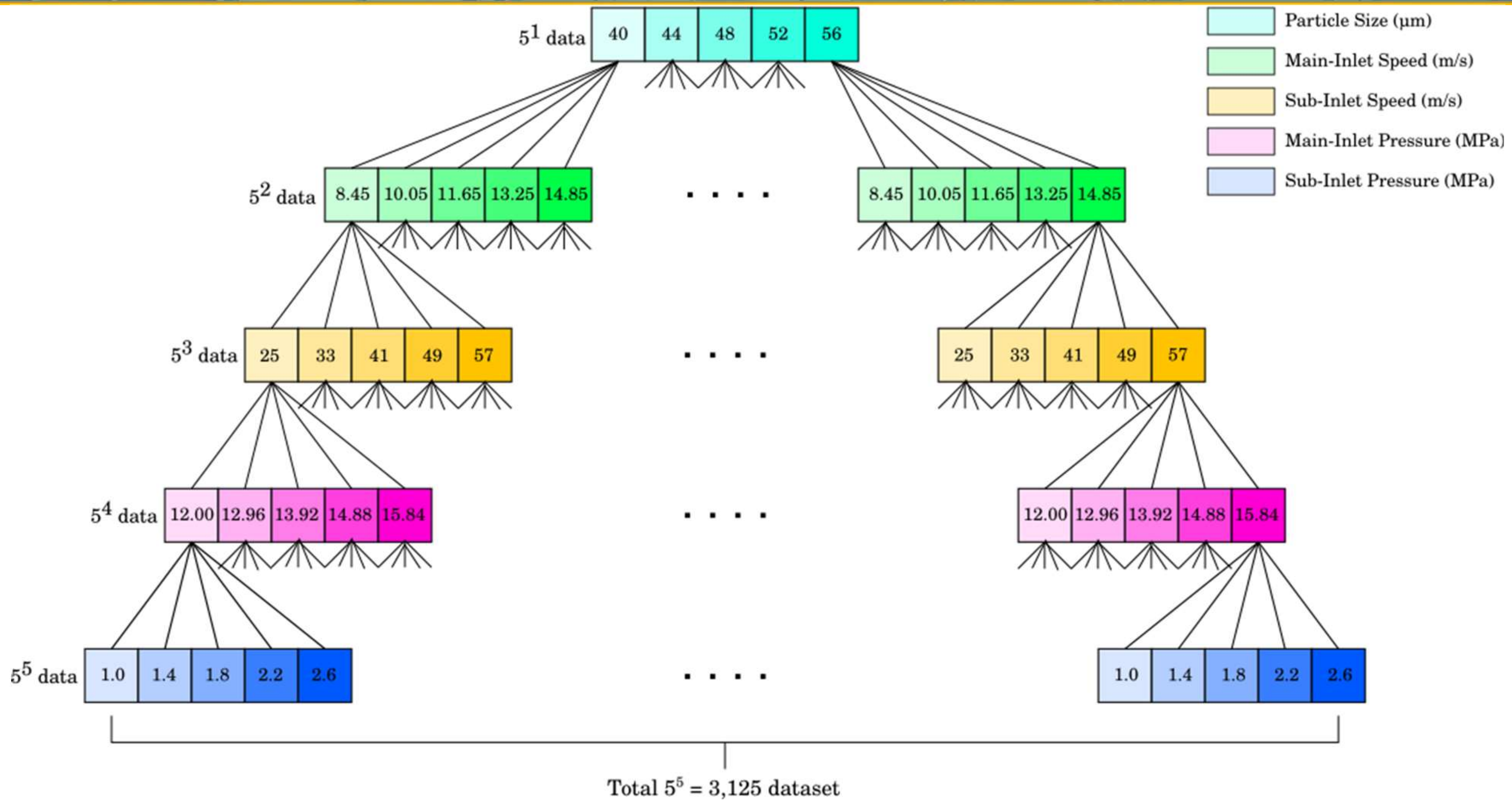
Erosion mechanism is directly related to trajectory of particle after collision on wall.



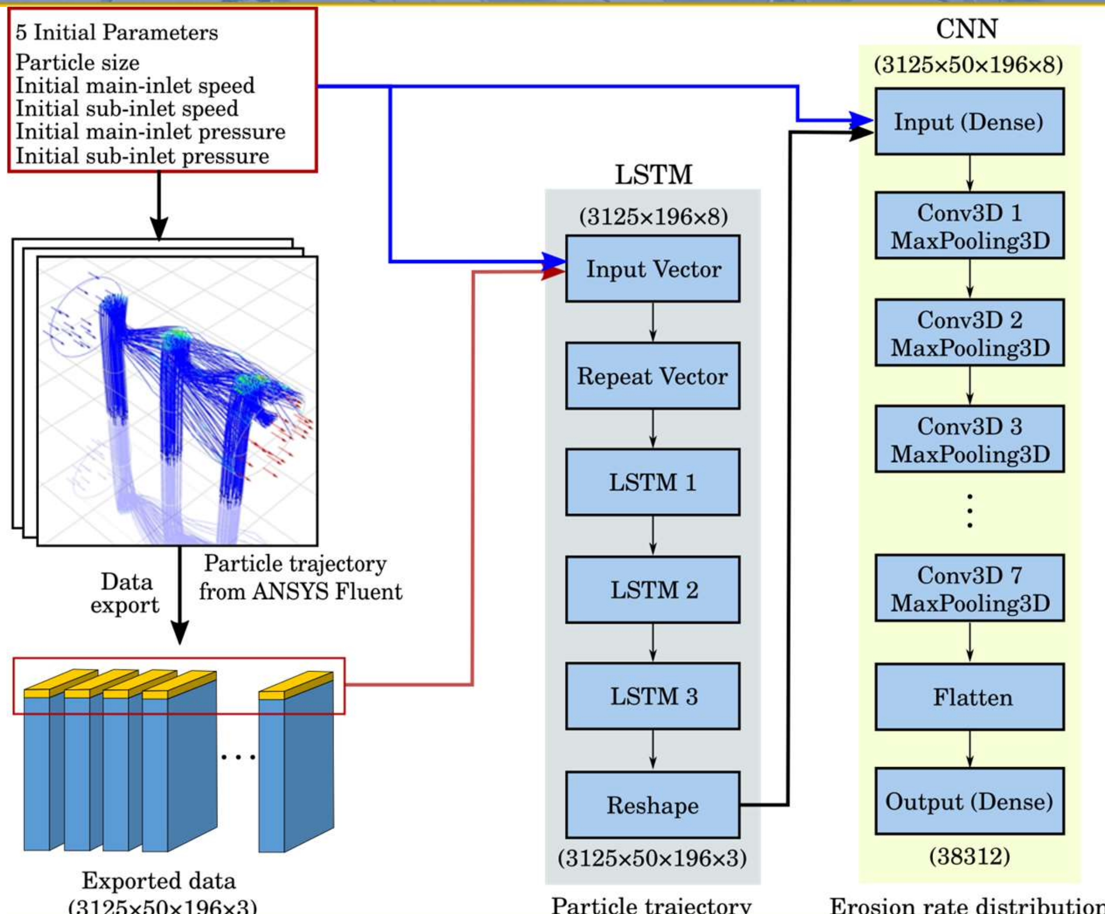




Simulation Running with Systematic Variable Control



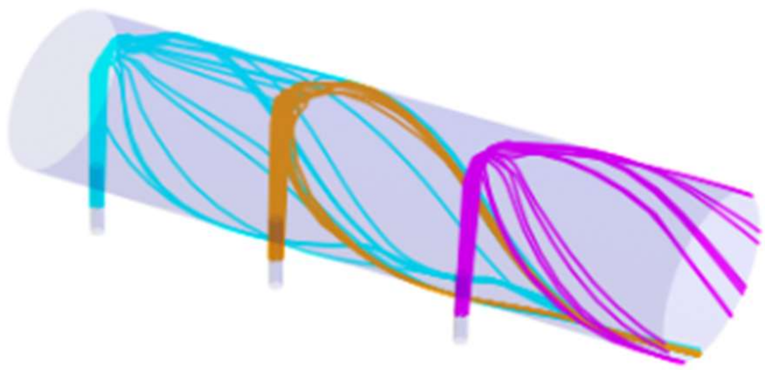
Workflow Diagram



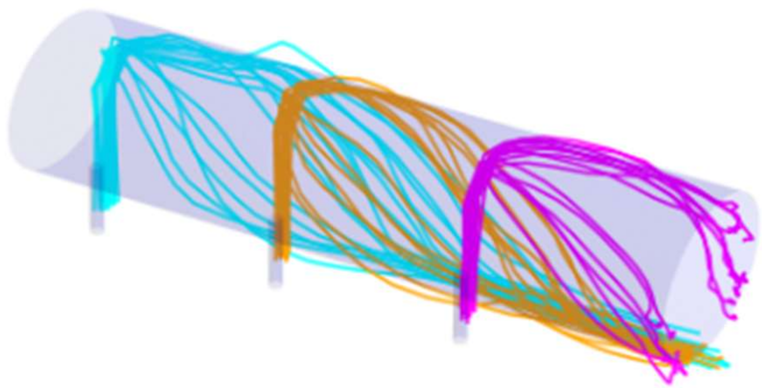
Results & Discussion

Particle Trajectory Results (Test Dataset)

Particle trajectory from CFD

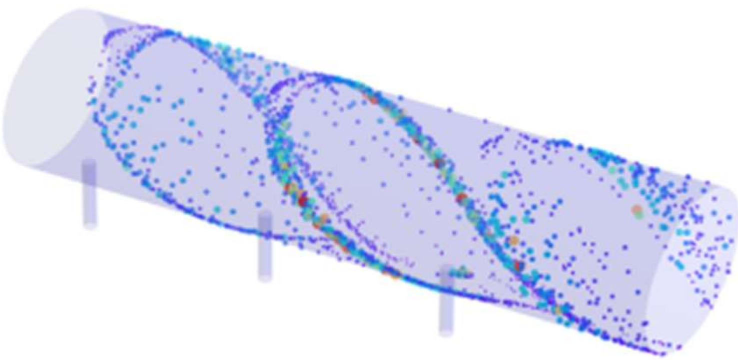


Particle trajectory from LSTM

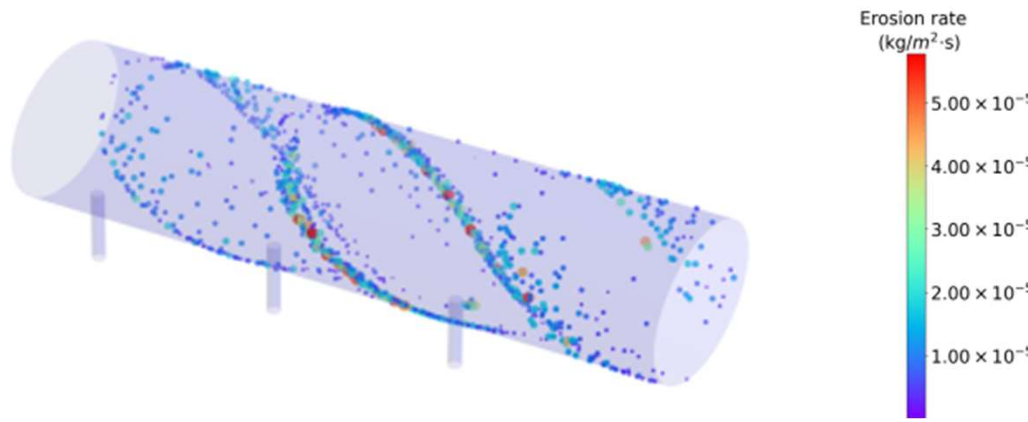


Erosion Rate Results (Test Dataset)

Erosion from CFD

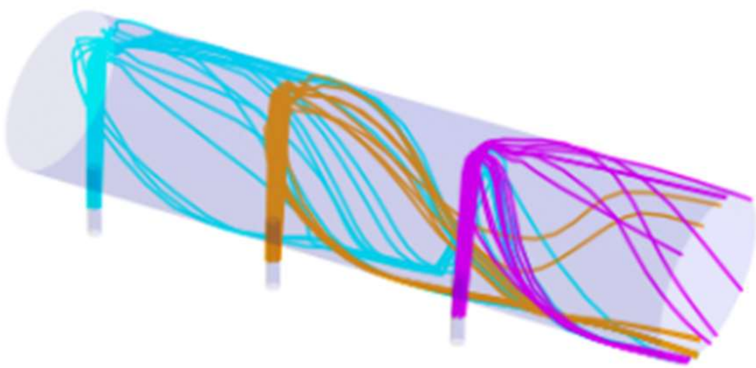


Erosion from LSTM+CNN

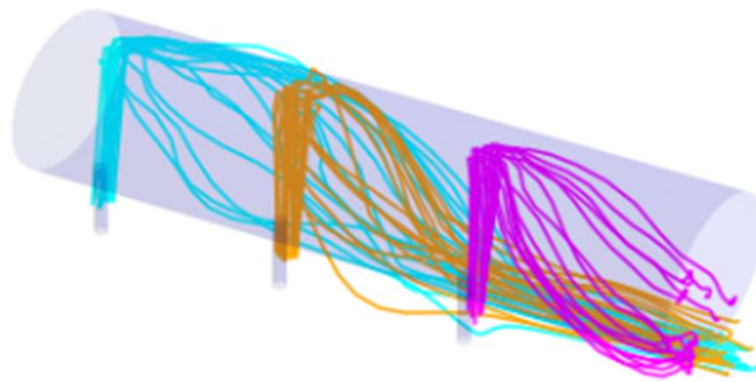


Particle Trajectory Results (Validation Dataset)

Particle trajectory from CFD

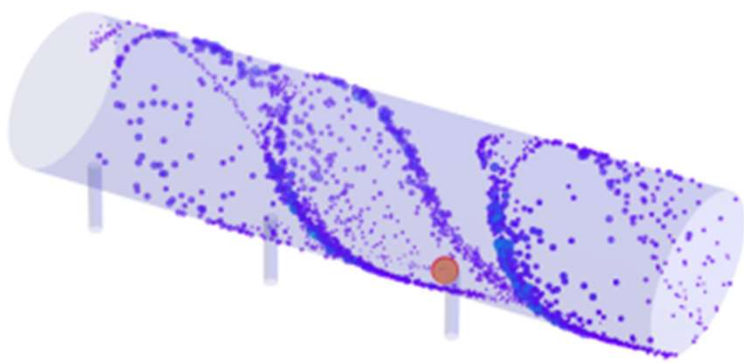


Particle trajectory from LSTM

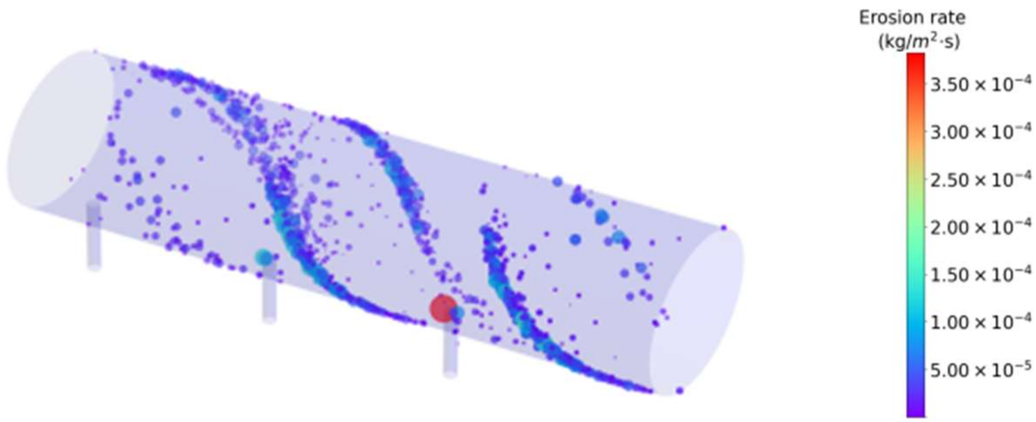


Erosion Rate Results (Validation Dataset)

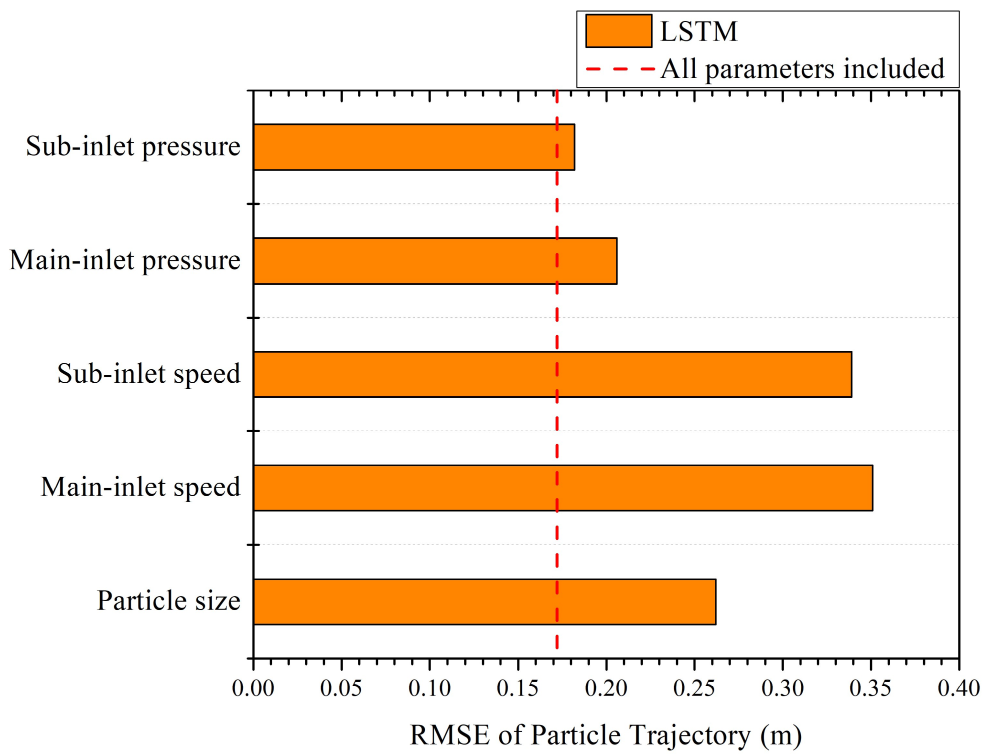
Erosion from CFD

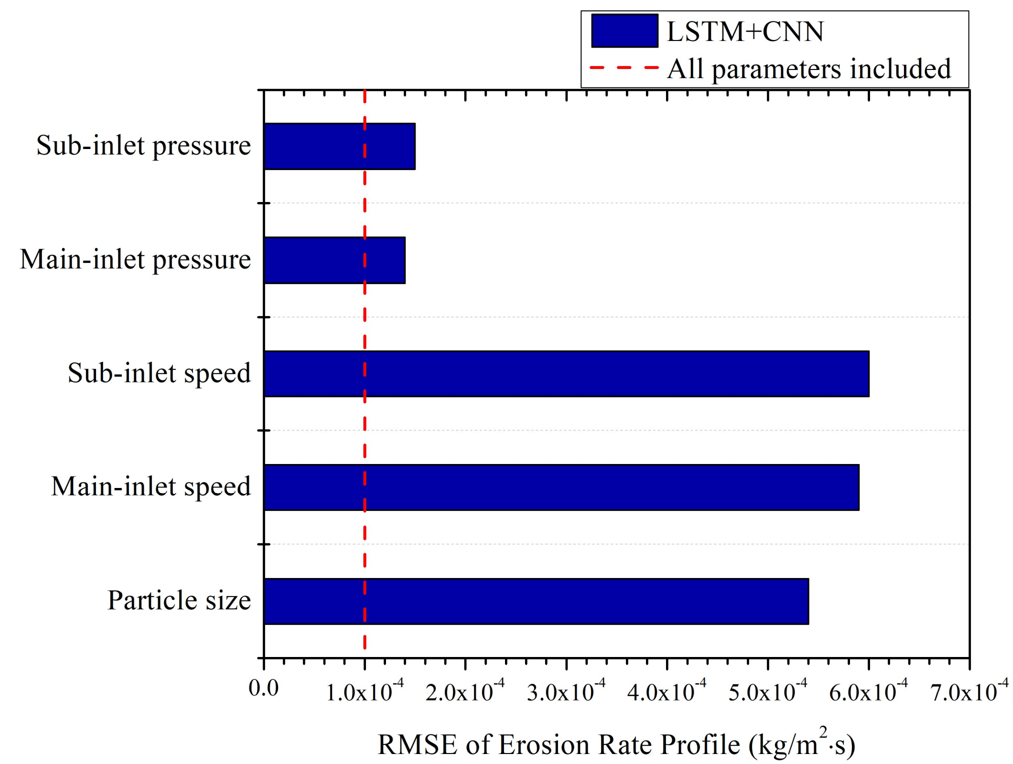


Erosion from LSTM+CNN

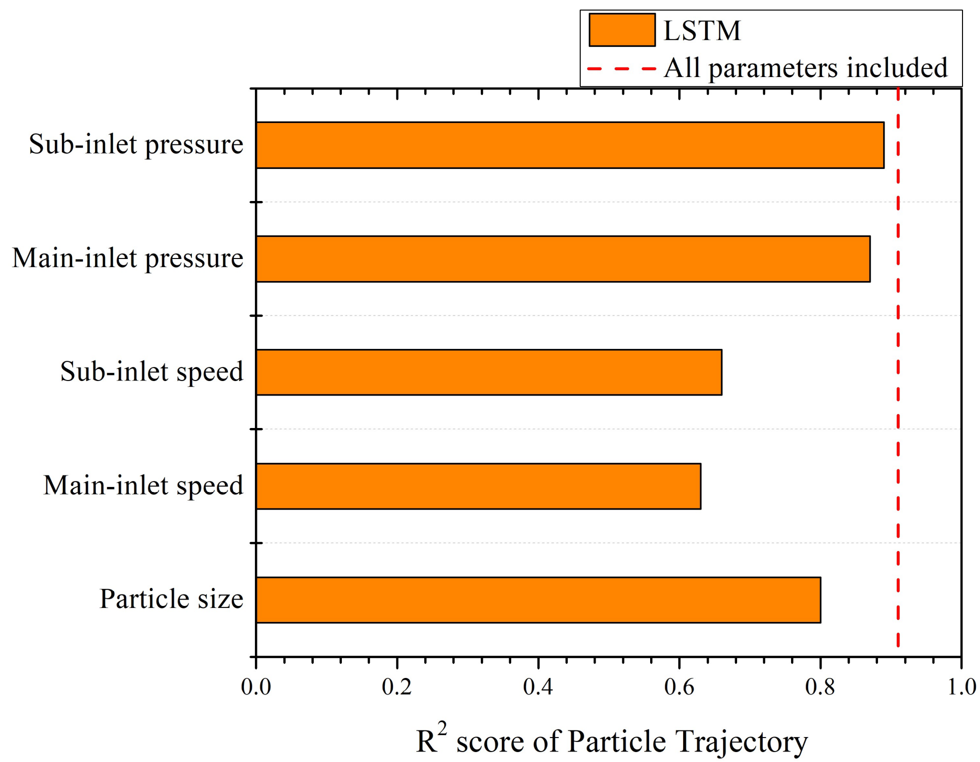


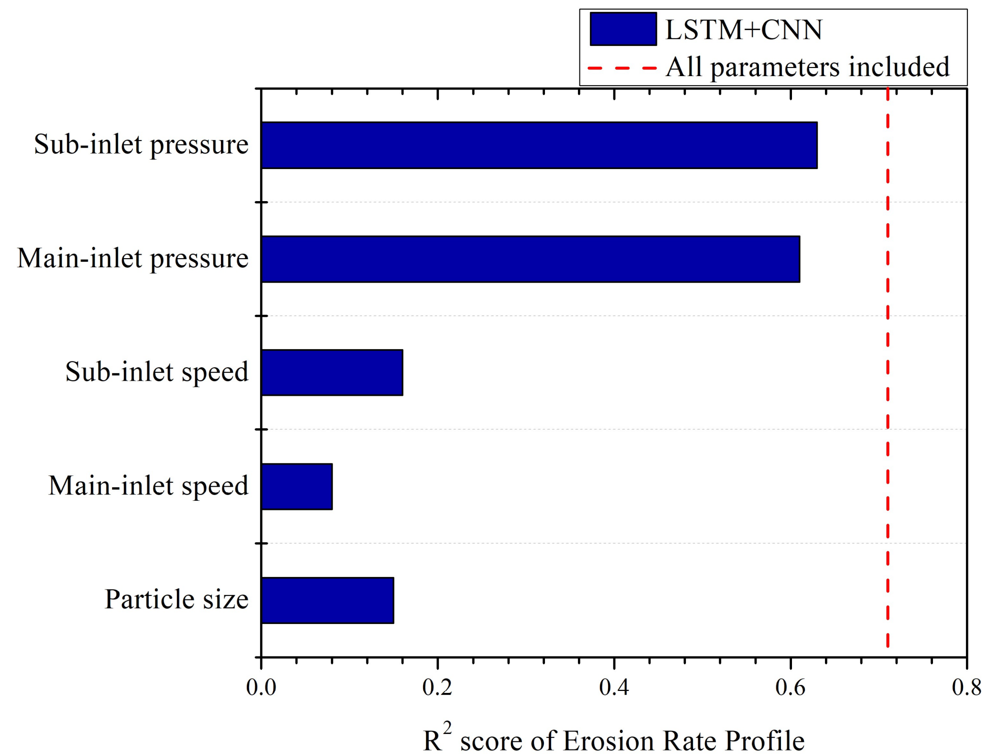
Feature Importance Analysis (RMSE)



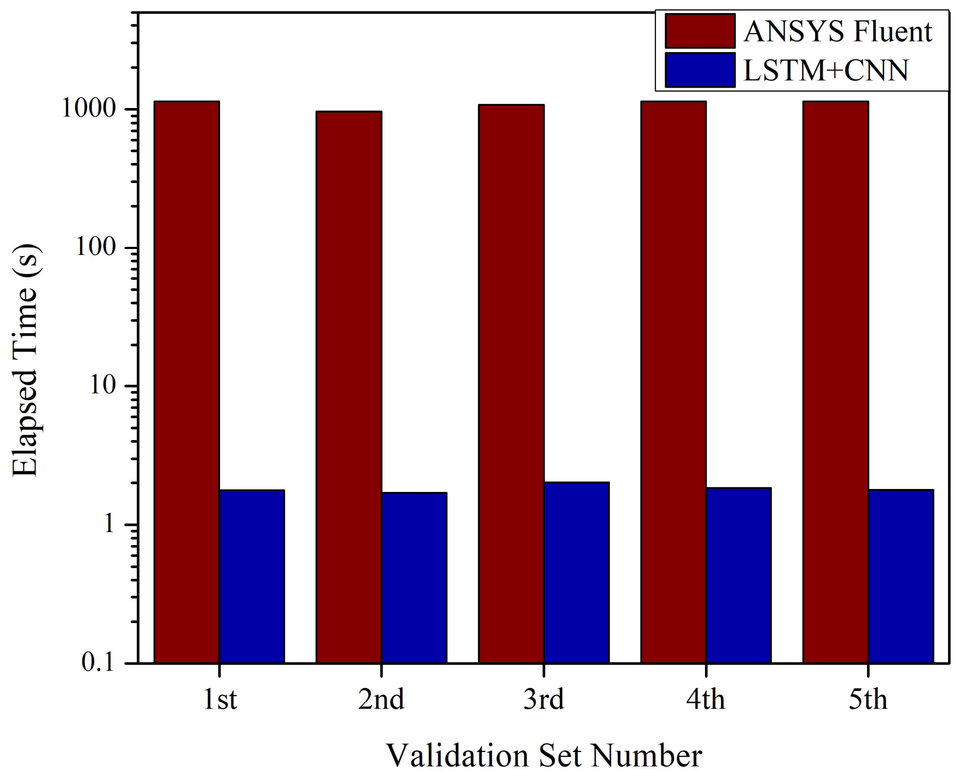


Feature Importance Analysis (R^2 score)





Computational Time Comparison between CFD & LSTM+CNN



Accomplishments

- 1. Provides new computational analysis (with LSTM + CNN hybrid model) to identify & develop insight into inefficiencies of specific physical processes in existing coal plants

- 2. Predicts damage rates of steam distribution header with Deep Learning neural network model
  1) Constructed LSTM model for particle trajectory prediction
  2) Developed CNN model to predict erosion rate profile
  3) Generated numerous datasets with changing system setup variables & fed data into LSTM + CNN layers to make high performing erosion prediction model.

Significance of Research

1. LSTM + CNN hybrid model for erosion prediction will skip entire iterative calculations of Reynolds-Averaged Navier Stokes equations on given geometry & turbulence model. – Significantly reduces computational time & expense.

2. Predicts particle trajectories first & erosion distribution afterwards to provide comprehensive insight into damage mechanisms in existing coal plants.

3. Only requires initial parameters; easy to utilize in current industrial fields.

Conclusion

- A hybrid deep learning model (LSTM + CNN) based on statistical analysis of CFD output parameters was developed & applied to simplified OP-650 steam distribution header for case study.
- Particle trajectory prediction was accomplished with LSTM model

  Average R^2 score: 0.91
  Average mean squared error: 0.0172 m
- Erosion distribution prediction was accomplished with CNN model

  Average R^2 score: 0.71
  Average mean squared error: 0.0001 kg/m²·s

- Initial inlet speeds are critical parameters; mean squared error of the model increased most when information of speed parameters is excluded.
- Our ML approach is over 600 times faster than numerically intensive CFD calculations & gives similar accuracy for predicting surface erosion rates but with significantly less computational time.

Acknowledgments & Disclaimer

This work was supported by the U.S. Department of Energy, National Energy Technology Laboratory (NETL) under Award DE-FE0031746.

CFD Particle tracking in a gas flow

1. Eulerian-Eulerian model

- Treats gas flow & solid phase as continuum
- Gas & particle phases treated as interpenetrating continua & coupled together by exchange coefficients

2. Eulerian-Lagrangian model

- Gas flow treated as continuous phase, but solid phase treated as dispersed phase
- Particle volume fraction usually assumed negligible compared to carrier phase volume & particle-particle interactions usually neglected

Eulerian-Lagrangian model is **Discrete phase modeling (DPM)** & was successfully demonstrated for various experimental cases. [1][2]

[1] Shankara, Prashanth S. *CFD simulation and analysis of particulate deposition on gas turbine vanes*. Diss. The Ohio State University, 2009.
[2] Peng, Z.; Doroodchi, E.; Moghtaderi, B. (2020). "Heat transfer modelling in Discrete Element Method (DEM)-based simulations of thermal processes: Theory and model development". *Progress in Energy and Combustion Science*. 79, 100847: 100847.

CFD Particle trajectory equation on DPM

- Particle trajectories obtained by integrating force balance equation written in Lagrangian reference frame given by

$$m_p \frac{dv_i^k}{dt} = \left(m_p - m_f\right) g_i + F_d^k .$$

v_i^k : k^{th} particles velocity in i^{th} direction

m_p : particle mass

m_f : fluid mass

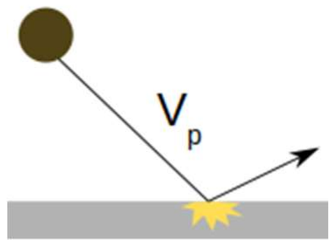
g_i : acceleration due to gravity

F_d^k : Stokes drag force acting on k^{th} particle due to relative velocity between fluid & particle

Factors affecting erosion under DPM

(1) Particle velocity

$ER \propto V_p^n$



V_p : particle velocity

Various values of n have been proposed

Finnie : n = 2
Oka : n = function of hardness

(2) Impingement angle

(3) Particle properties (hardness, size, shape, etc.)

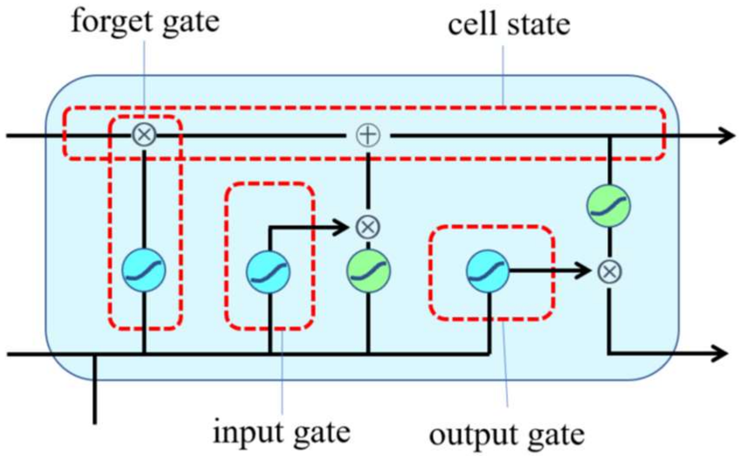
Oka & McLaury developed erosion models incorporating particle properties

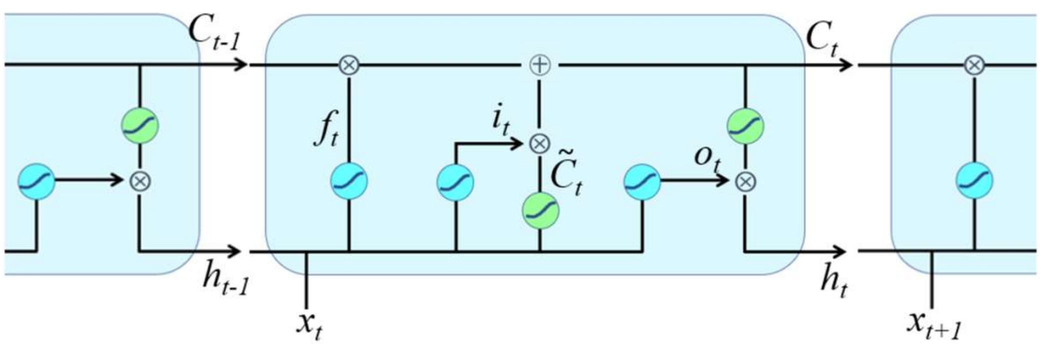
General formulation under DPM

$$ER = \sum_{p=1}^{N_{traject}} \frac{\dot{m}_p C(d_p) f(\alpha) v_p^n}{A_{face}}$$

m_p : ***Mass flow rate of the particles***
$f(\alpha)$: ***Impact angle*** function
v_p : ***Particle impact velocity***
n : Velocity exponent
$C(d_p)$: ***Particle diameter*** function

How LSTM works?





- LSTM approach utilizes chain-like structure with series of connected LSTM units. These units detect features from input sequence & attempt to learn long-term dependencies.
- LSTM unit consists of cell state & three gates that regulate information flow: a forget gate, an input gate, & an output gate.

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f),$$

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i),$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C),$$

$$C_t = f_t \cdot C_{t-1} + i_t \cdot \tilde{C}_t,$$

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o),$$

$$h_t = o_t \cdot \tanh(C_t),$$