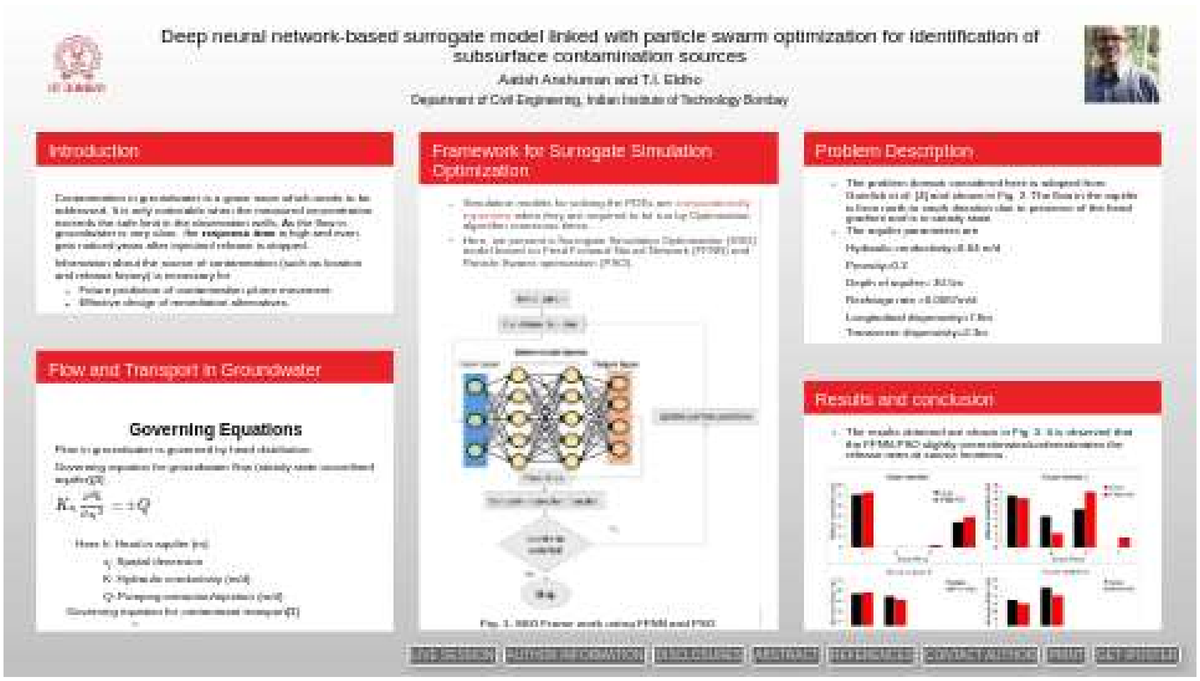
Deep neural network-based surrogate model linked with particle swarm optimization for identification of subsurface contamination sources



Aatish Anshuman and T.I. Eldho

Department of Civil Engineering, Indian Institute of Technology Bombay

PRESENTED AT:

INTRODUCTION

Contamination in groundwater is a grave issue which needs to be addressed. It is only noticeable when the measured concentration exceeds the safe limit in the observation wells. As the flow in groundwater is very slow, the **response time** is high and even gets noticed years after injection/release is stopped.

Information about the source of contamination (such as location and release history) is necessary for

- Future prediction of contamination plume movement.
- Effective design of remediation alternatives.
- Delineating the contaminated aquifer.

FLOW AND TRANSPORT IN GROUNDWATER

Governing Equations

Flow in groundwater is governed by head distribution.

Governing equation for groundwater flow (steady state unconfined aquifer)[3]

$$K_{x_i}\frac{\partial^2 h}{\partial {x_i}^2} = \pm Q$$

Here h: Head in aquifer (m)

x_i: Spatial dimension

K: Hydraulic conductivity (m/d)

Q: Pumping extraction/injection (m/d)

Governing equation for contaminant transport[3]

$$\frac{\partial c}{\partial t} = D_{xx_i}\frac{\partial^2 c}{\partial {x_i}^2} - v_{x_i}\frac{\partial c}{\partial x_i} + Q$$

Here c: contaminant concentration (ppm or, mg/L)

t: Time

x_i: Spatial dimension

D: Dispersion coefficient (m2/d)

v: Seepage velocity(m/d)

Q_c: Contaminant injection (ppm/d)

The PDEs (Partial Differential equations) are required to be solved in the problem domain for computation of head and concentration distribution.

Radial Point Collocation Method

A meshfree numerical method named Radial Point Collocation Method (RPCM) is used for solving the PDEs as it is more advantageous compared to grid/mesh based methods such as Finite Difference Method and Finite Element Method [2].

The PDEs are discretized in the domain using shape functions which are estimated using Multiquadrics radial basis function.

FRAMEWORK FOR SURROGATE SIMULATION OPTIMIZATION

- Simulation models for solving the PDEs are computationally expensive when they are required to be run by Optimization algorithm numerous times.
- Here, we present a Surrogate Simulation Optimization (SSO) model based on Feed Forward Neural Network (FFNN) and Particle Swarm optimization (PSO).

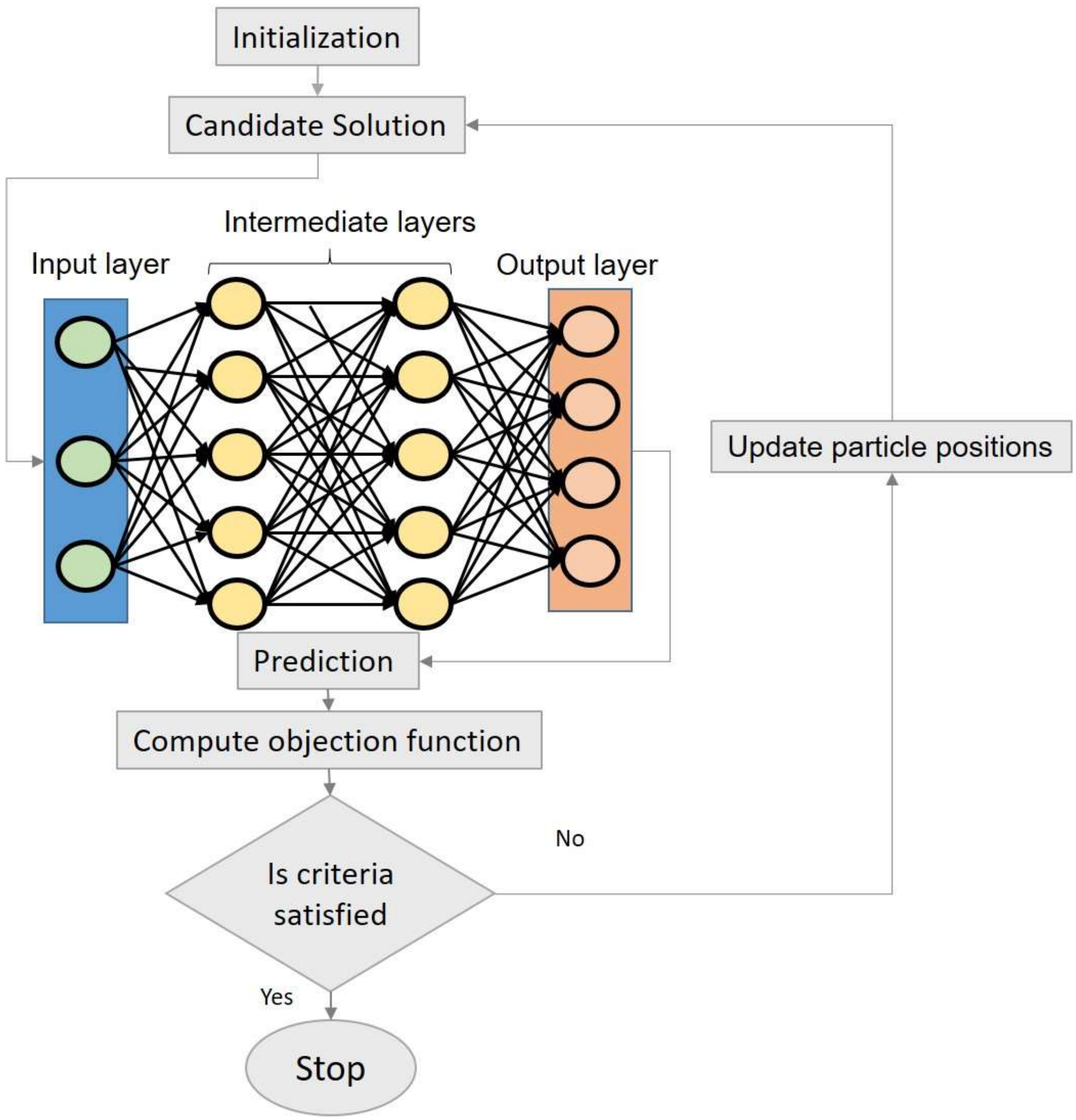


Fig. 1. SSO Frame work using FFNN and PSO

- FFNN is a type of DNN which has more than one intermediate layers. In this study, FFNN is developed using Tensorflow [1].
- The input data for FFNN is release rates at source and output data is the concentrations at the observation wells as simulated by RPCM model. FFNN is fit using ADAM optimization technique.
- The fitted FFNN model is embedded within PSO which updates the candidate solution based on the objective function/loss function value.

- PSO algorithm mimics the swarm behaviour of a bird flock [5]. The population of the swarm is assigned a velocity which is updated at every iteration as per the following formula.

$$v_i^{t+1} = \omega.\, v_i^t + c_1.\, r_1.\, (p_{best} - x_i^t) + c_2.\, r_2.\, (g_{best} - x_i^t)$$

Here **ω,** C_1 and C_2 are PSO model parameters

r_1 and r_2 are random numbers between 0 and 1

p_{best} is the best position of ith particle

g_{best} is the best position of the swarm

$\mathbf{v_i^t}$ is velocity of the ith particle for iteration number t

- The objective/loss which is required to be minimized by PSO is given by

$$\frac{1}{n}\sum_{i=1}^{n}\left(c_{sim}^{i} - c_{obs}^{i}\right)^2$$

Here $\mathbf{c^i_{sim}}$ and $\mathbf{c^i_{obs}}$ are surrogate model simulated concentrations and observed concentrations.

PROBLEM DESCRIPTION

- The problem domain considered here is adopted from Gorelick et al. [4] and shown in Fig. 2. The flow in the aquifer is from north to south direction due to presence of the head gradient and is in steady state.
- The aquifer parameters are

  Hydraulic conductivity=8.64 m/d

  Porosity=0.2

  Depth of aquifer= 30.5m

  Recharge rate =0.0067m/d

  Longitudinal dispersivity=7.6m

  Transverse dispersivity=2.3m

- There are 5 possible contamination sources around the pond which inject total dissolved solids into aquifer for 4 years.
- The observation wells (OB_1, OB_2 and OB_3) are located in the aquifer which measure TDS concentrations for over 15 years. Since, the concerned problem is hypothetical, the RPCM

simulated concentrations are treated as observed concentrations.

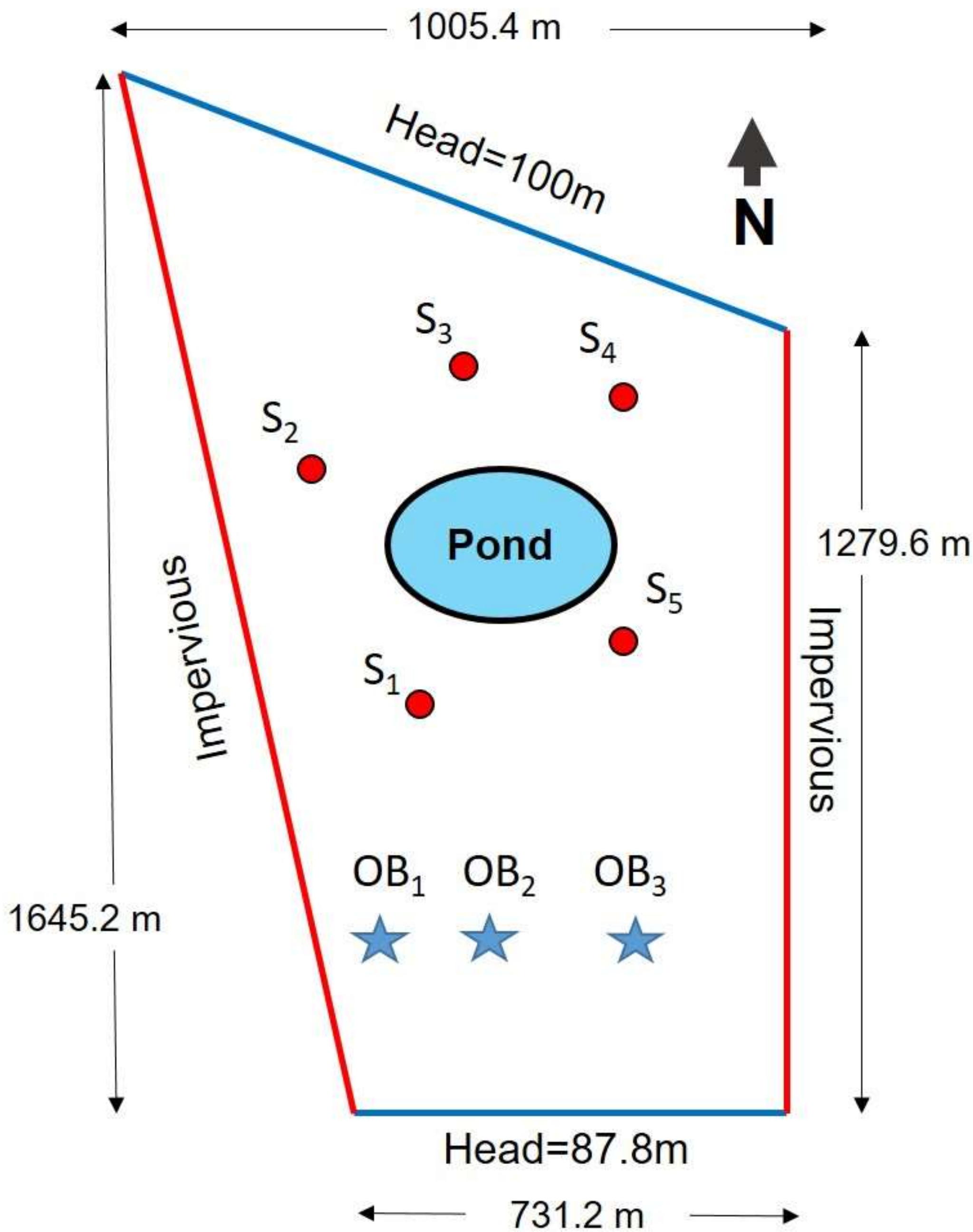


Fig. 2. Schematic diagram of the study area (modified from Gorelick et al. [4])

- The FFNN model is fitted using normalized release rates at the possible source locations for 4 years as input and normalized RPCM simulated concentrations at observed well for 15 years as output.
- The fitted FFNN model is linked with PSO which tries different candidate solutions and minimizes the objective function. The FFNN-PSO is run for 1000 iterations with a population size of 200. Here, the maximum number of iterations i.e. 1000 is selected as stopping criteria.

RESULTS AND CONCLUSION

- The results obtained are shown in Fig. 3. It is observed that the FFNN-PSO slightly overestimates/underestimates the release rates at source locations.

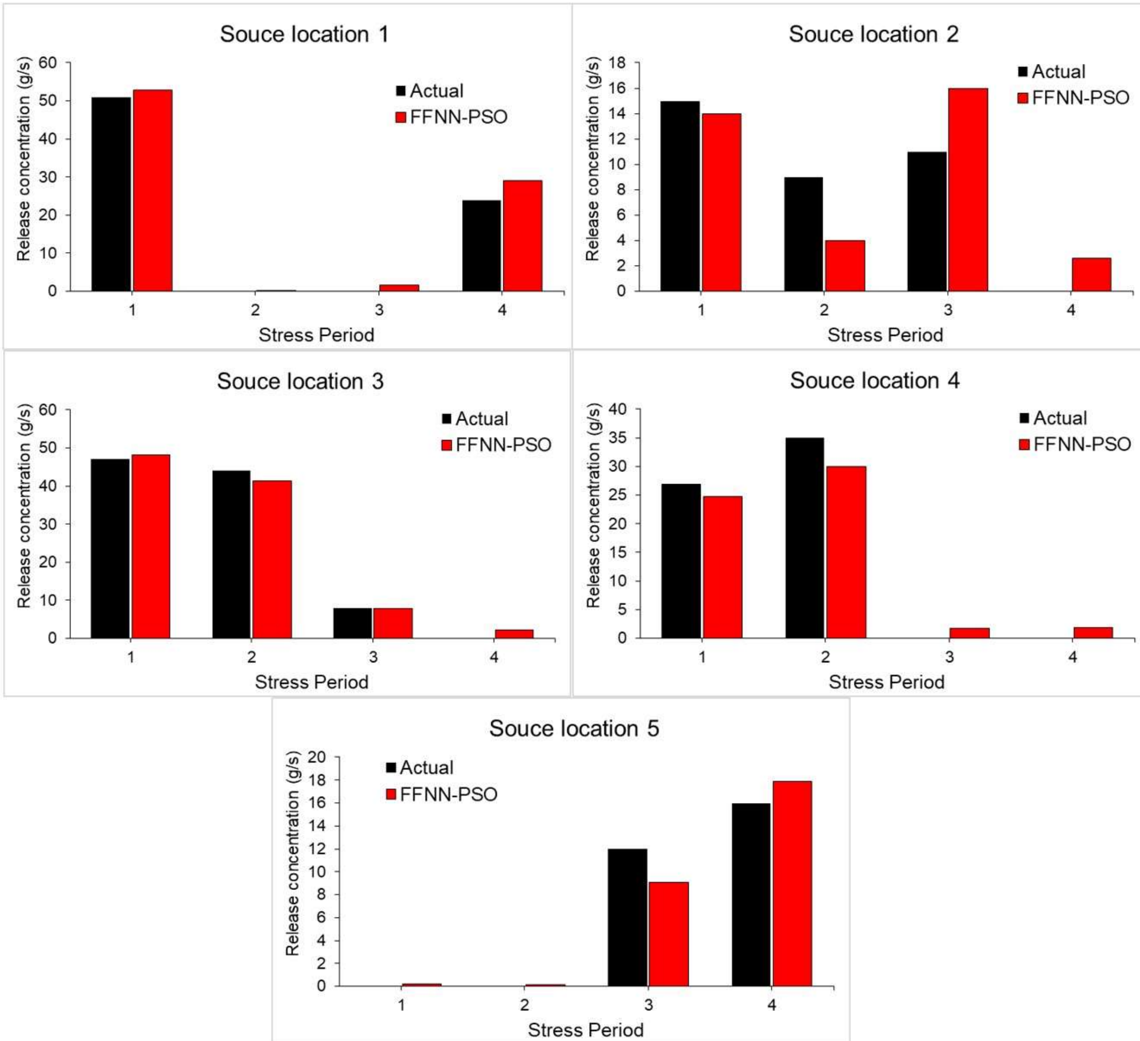


Fig. 3. Comparison of actual and predicted concentrations at different source locations

- The root mean squared error (RMSE) and coefficient of determination (R^2) obtained are 2.75 and 0.97 which indicates that the FFNN-PSO model can be considered as satisfactory.

- From the comparison of results obtained using linear programming (LP) and stepwise regression (SR) available in the literature [4], it is observed that RMSE values for LP and SR are 1.36 and 2.72 respectively. Similarly, R^2 values for LP and SR are 0.99 and 0.97 respectively.

- The time taken for the FFNN model for one simulation is 0.0015 seconds compared to 2.78 seconds in RPCM. This is the major advantage of the SSO technique which allows for large population size in the optimization algorithm thus ensuring faster convergence.

- Accuracy SSO technique depends on the accuracy of the surrogate model. The FFNN model interprets the input data as vector and provides the output data in form of a vector due to which the important information about the categorization of sources and temporal dimensional is not taken into consideration.

- The performance of the SSO technique may be improved by using other neural network architectures such as Recurrent Neural Networks (RNN) which deals with this issue effectively.

DISCLOSURES

Acknowledgements

The authors thank the Board of Research in Nuclear Sciences (BRNS) for providing support through the project “Modelling of reactive transport in groundwater using meshfree based numerical methods” (Project no. 16BRNS002).

AUTHOR INFORMATION

Aatish Anshuman is a PhD research scholar n the Department of Civil Engineering, IIT Bombay.

T.I. Eldho is a Proffessor in the Department of Civil Engineering, IIT Bombay.

ABSTRACT

Identifying subsurface contamination is challenging as the sources are not directly perceivable. Aquifer contamination only gets noticed when it is measured in one of the observation wells. As remediation of the contaminated sites is expensive and time-consuming, it is essential to locate sources of contamination for efficient remediation design and water resources management. Simulation-optimization approach is popularly used for identification of contaminant sources. However, the numerous runs required for the simulation model by utilizing the optimization algorithm makes this approach computationally expensive. Alternatively, the simulation model can be substituted by a surrogate model which can significantly reduce the computational cost. In this study, a deep neural network (DNN) based surrogate model is proposed for simulating the transport of a reactive contaminant Tritium in a hypothetical aquifer. The DNN is trained by considering injection rates at possible source locations as inputs and concentration at observation wells simulated by meshfree Radial Point Collocation Method (RPCM) as output. RPCM efficiently handles instabilities associated with advection and reaction dominant problems in comparison to grid/mesh-based methods. The backpropagation approach is used to optimize the weights and biases of the DNN using adaptive moment estimation (ADAM) as an optimizer. The performance evaluation of the surrogate model yields Mean Squared Error (MSE) close to zero and correlation coefficient (R^2) of 0.99. An inverse model is developed by linking the DNN surrogate model and Particle Swarm Optimizer (PSO). The application of the inverse model show that the DNN-PSO model can predict the injection rates at possible source locations accurately.

REFERENCES

1. Abadi, M., Barham, P., Chen, J., Chen, Z., Davis, A., Dean, J., & Kudlur, M. (2016). Tensorflow: A system for large-scale machine learning. In 12th USENIX symposium on operating systems design and implementation (OSDI 16) (pp. 265-283).
2. Anshuman, A., Eldho, T. I., & Singh, L. G. (2019). Simulation of reactive transport in porous media using radial point collocation method. Engineering Analysis with Boundary Elements, 104, 8-25.
3. Bear, J., & Cheng, A. H. D. (2010). Modeling groundwater flow and contaminant transport (Vol. 23). Springer Science & Business Media.
4. Gorelick, S. M., Evans, B., & Remson, I. (1983). Identifying sources of groundwater pollution: An optimization approach. Water Resources Research, 19(3), 779-790.
5. Kennedy, J., & Eberhart, R. (1995, November). Particle swarm optimization. In Proceedings of ICNN'95-International Conference on Neural Networks (Vol. 4, pp. 1942-1948). IEEE.