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Use of Neural Networks to Model the Radiative Transfer Equation for a Domain with Participative Gases

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Abstract

This paper focuses on the modelling of the radiative transfer equation in a 2-D walled domain with participative gases. Aiming to reduce the computational cost of the physical resolution, a neural network-hybrid approach is introduced to model the radiative transfer equation. The solution of the radiative transfer equation is learned through two multi-layer perceptron networks whose inputs are the wall temperatures and the length and the temperature of the domain elements, and whose outputs are radiation intensities and transmissivities. To validate the approach, the results are compared with those of a proven in-house physical radiation solver in which the discrete transfer ray method is used to numerically solve radiative transfer equation with participative gases. To model the spectral behaviour of gases, the physical solver uses the spectral narrow band model with the Curtis-Godson modification. The dependency of the wall emissivity with the spectral wavelength was neglected.

The approach was tested for a typical hydrocarbon combustion, at constant atmospheric pressure, with a range of wall and gas temperature between 300K to 3000K, for a fixed CO_2 to H_2O molar ratio. Comparison between the neural network hybrid approach and the physical solver are presented. For an academic use case discretized over 5 cells, precision of the hybrid approach shows a relative error under 3% with a speed-up factor around 10. First results are rather promising in terms of wall heat fluxes. The model could be extended by varying the gas composition and/or pressure.

Keywords: thermal radiation, participative gases, radiative transfer equation, discrete transfer ray method, statistical narrow band, machine learning, neural network

1 Introduction

The accuracy and the numerical cost of simulating radiative heat transfer is strongly related to the choice of mathematical model, discretization methods and the assumptions made regarding the behaviour of the participative gases. The high cost is related to the resolution of the Radiative Transfer Equation (RTE), which implies both a spatial and an angular integration [1]. An additional difficulty comes from the fact the gas behaves as a non-transparent medium in which the transmissivity depends on the wavelength. Indeed, combustion products such as carbon dioxide and steam act as participative gases to the radiation, either by absorbing or emitting radiant energy.

Proposed by Lockwood and Shah [2], the Direct Transfer Radiative Method (DTRM) is used for its acceptable compromise between accuracy and computational cost. The DTRM solves representative rays in discretized space directions that need to cover the entire domain.

When the spectral aspects are considered, an additional discretization over the wavelengths has to be done. Then, the spectral dependency of the participative gases and walls has to be taken into account. One way to calculate the transmissivity of each spatial element is to use the Statistical-Narrow-Band (SNB) model [3] with the Curtis Godson (CG) modification [4, 5].

In this work, only the dependency of the gases parameters with the spectral wavelength is considered. The emissivity of the walls is averaged over the infrared spectrum. The solution of the RTE using DTRM for a domain with participative gases is implemented in an in-house FORTRAN solver co-developed by Air Liquide [6] and the EM2C laboratory [7] in the 90's. This solver is considered to provide high-fidelity solutions and therefor it will be used as reference.

The principal limitation of the spectral methods is an unaffordable computational cost for most industrial applications. The aim of the current work is to advantageously use neural network techniques, more precisely the Multi-Layer Perceptron (MLP) to model the radiative transfer faster while maintaining main spectral aspects.

2 Methods

Here, the steady-state radiative transfer equation for a participative, non-scattering gas is considered. The transmissivity of a gas column is calculated based on SNB model with CG modification.

The DTRM is used to spatially discretize the RTE. The intersection between a ray and the meshed domain results in a division of the ray in several elements (see Figure 1). Note that different rays cross a different number of cells, which leads to a wide range of element lengths.

It is worth mentioning that the radiative intensities are dependent of spectral wavelength in the infrared spectrum. The SNB discretizes this spectrum over wavenumber bands of 25 cm^{-1}.

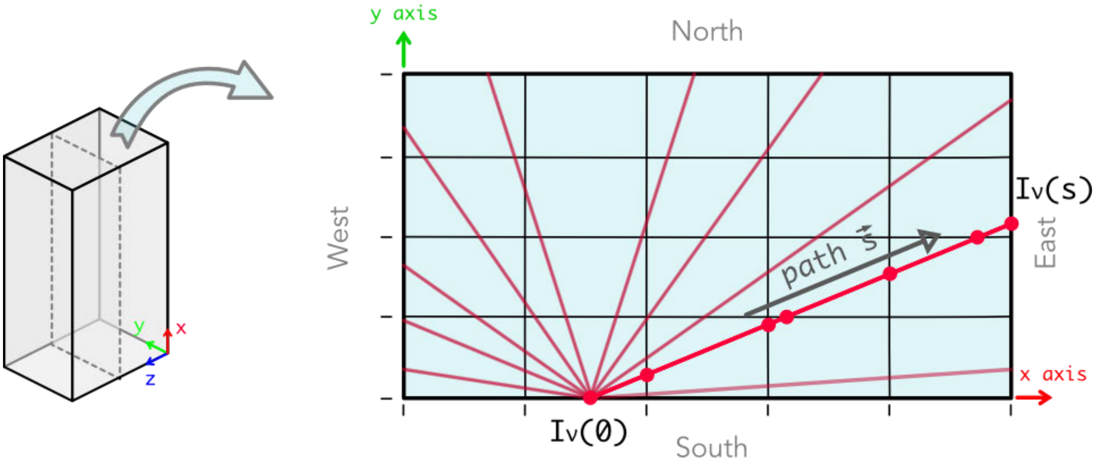

Figure 1. Spatially meshed domain with rays shot in various angular directions from a specific point of the boundary.

The aim of the present study is to accelerate the calculation of the radiative intensities. By use of machine learning, a strategy is proposed to include the spectral dependency without explicitly computing it. To do that, the radiative intensities and specific mean transmissivities of rays are modelled by two neural networks. Note that, although the specific mean transmissivities have the same meaning, they are not actual transmissivities.

Figure 2 illustrates the parameters of interest for a representative ray that starts from a wall point and arrives on an ending wall by passing through 6 elements. This representative ray is also highlighted in Figure 1.

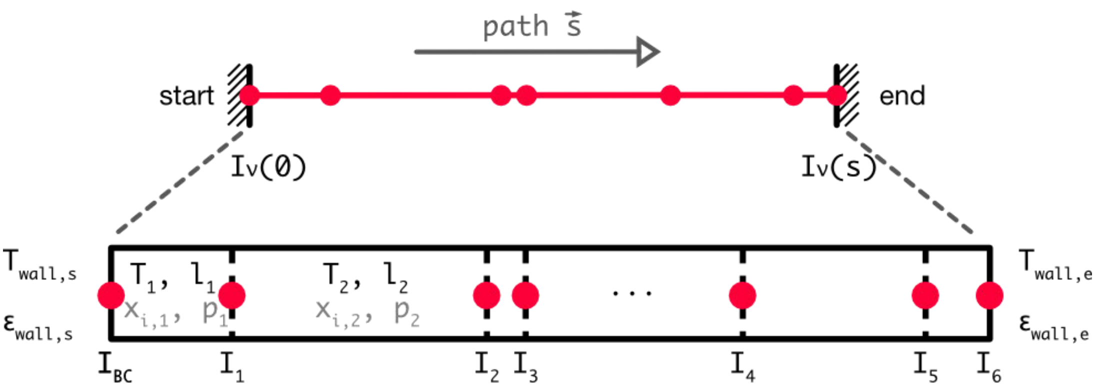

Figure 2. Illustration of a representative radiative ray described by the temperature and emissivity of walls, the temperature, composition, pressure and length of each element.

These parameters are the input parameters of two neural networks. For the first one, the outputs is the radiative intensities, while for the second one, the outputs is the specific mean transmissivities. These neural networks can be used to substitute the solver's module where the intensities and the transmissivities are computed traditionally. In summary, to solve the RTE with the hybrid model, one needs to:

- discretize the domain spatially, and set the gas parameters for each spatial element,
- draw rays from each point from the boundary,
- use the MLPs to predict the radiative intensities of each ray,
- for each boundary point, sum all the incident rays contribution

The advantage of the proposed model is that these learned rays can be used to calculate the radiative intensities for any type of geometry.

3 Results

Firstly, a typical ray with 20 elements was considered. The temperatures and lengths of the ray vary from 300K to 3000K, and $2x10^{-4}$m to 2m, respectively. The molar fractions chosen are 0.194 for H_2O and 0.182 for CO_2. The remaining molar fraction is N_2, a non-participative gas. The pressure in the domain is constant at 1 atm. The emissivity for the furnace walls was set to 0.25.

50k input samples (wall temperature, length, and temperature of the domain elements) for training and 10k input samples for testing the neural networks were generated using the latin hypercube method. These inputs were given to another physical solver developed specifically for the ray samples. This solver gives the output samples (radiative intensities and specific mean transmissivities) for training and testing the two MLPs. In what followed, two MLPs were trained to predict the radiative intensities and the specific mean transmissivities, respectively. It is worth noting that the inputs and outputs of the MLPs were normalized.

Tables 1 summarize the hyper-parameters that were chosen for the two MLPs to predict the radiative intensities and the specific mean transmissivities of the sampled rays, respectively.

Parameter	Radiation intensities	Specific mean transmissivities
Architecture	1 hidden layer with 1025 neurons	3 hidden layers with 998/926/1532 neurons
Activation functions	ReLu	Linear/ReLu/ReLu
Epoch number	350	
Batch size	50	1076
Validation split	25%	
Loss Function	Mean Absolute Error	
Optimizer	Adam (learning rate = 0.0005)	
Normalization	True	

Table 1: Hyper-parameters of the MLP for prediction.

The mean average error for the training and cross-validation of the predicted radiative intensities and the specific mean transmissivities are shown in Figures 3 and 4. The mean average errors for the unseen test samples are 0.02 and 0.05 for radiative intensities and specific mean transmissivities, respectively. These MLPs replace the solver's module.

The neural network-hybrid approach for modelling and solving the RTE was tested in a 2-D domain. The domain is a 1mx1m rectangular box. The vertical and horizontal boundaries were equally divided in 5. From the centre of each wall cell, 20 rays are shot in equally angular directions. The typical elements size of rays being $1x10^{-3}$m to $3x10^{-1}$m. For the following use case, the temperature of the walls and the gases are 2500K and 1500K, respectively.

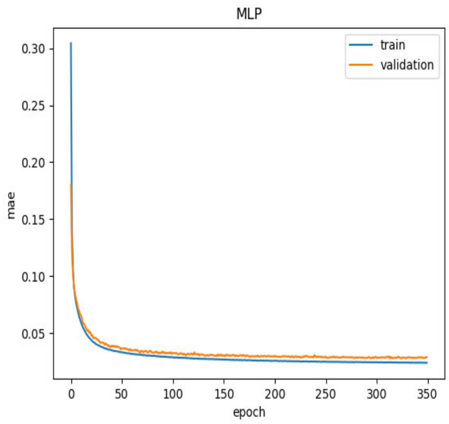

Figure 3. Mean average error for the training and cross-validation of the radiation intensities

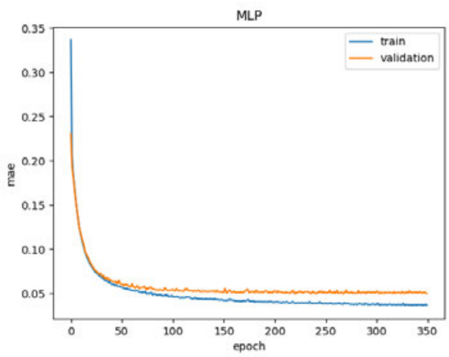

Figure 4. Mean average error for the training and cross-validation of the specific mean transmissivities

The MLP for prediction of the radiative intensities is used for a case where the reflective contributions of the incident radiative intensities are neglected. The results are shown in Figure 5. For this case, the relative error is under 1%, which validate the corresponding MLP training.

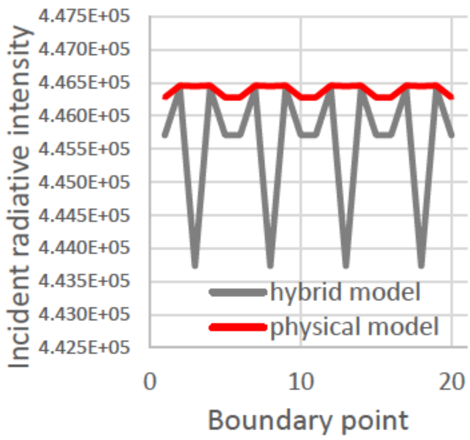

Figure 5. Comparison between physical and hybrid solver for neglected reflective contributions

For the case where the reflective intensities are considered, both MLPs have to be used to predict the incident radiative intensities. The results are depicted in Figure 6. In this case, the relative error is under 3%.

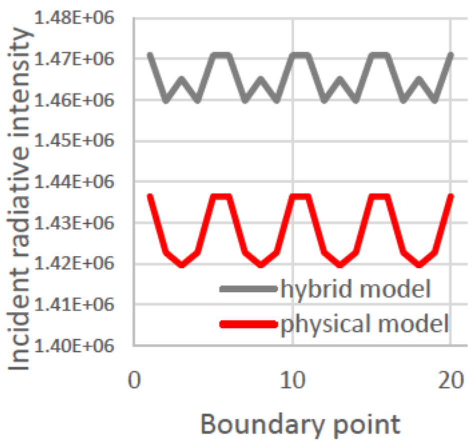

Figure 6. Comparison between physical and hybrid solver including reflective contributions

For this case, the net computational time of the hybrid approach was almost 10 times faster than the physical solver.
Further studies should be done to validate this approach on various physical and geometrical parameters.

4 Conclusions and Contributions

The current work showed how to advantageously use neural network techniques for modelling the radiative transfer equation while taking into account the spectral behaviour of the participative gases. The concept introduced is that the total radiative intensity along rays can be modelled by MLPs.

Latin Hyper Cube sampling technique was used to generate a multitude of rays with varying parameters of interest: temperature for the walls and length and temperature for each element of the spatial domain. The wall emissivity, the composition and pressure of the elements were kept constant and chosen in accordance to typical combustion flue gases (CO_2 and H_2O).

Then, these input samples were used to calculate the radiative intensities at the boundaries for each ray element using an in-house classical solver in which DTRM with SNB-CG is implemented. In addition, specific mean transmissivities were calculated. These calculated radiative intensities and specific mean transmissivities were used as the outputs for training two MLPs. In what followed, these learned rays were used to predict the incident radiative intensities on the boundaries. A 2-D rectangular geometry (1m x 1m) was considered with the wall temperatures 2500K and the gas temperature 1500K. The predicted incident radiative intensities were in good agreement with those calculated by the physical solver. The hybrid solver was 10 times faster than the physical solver.

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