# Detonation Cell Size Measurement and Prediction for Hydrogen- and Hydrocarbon-Nitrous Oxide Mixtures

Georgios Bakalis[1], Bo Zhang[2] and Hoi Dick Ng[1]
1. Department of Mechanical, Industrial and Aerospace Engineering, Concordia University, Montreal, Quebec, H3G 1M8, Canada
2. School of Aeronautics and Astronautics, Shanghai Jiao Tong University, Shanghai 200240, China

## 1 Introduction

Nitrous oxide ($N_2O$) has been used in a variety of industrial applications and is considered a relatively safer oxidizer to store and carry on board in a rocket motor engine. Like with oxygen, $N_2O$ mixed with other gaseous fuels can result in an explosion risk potential and prompt for the occurrence of detonation [1].

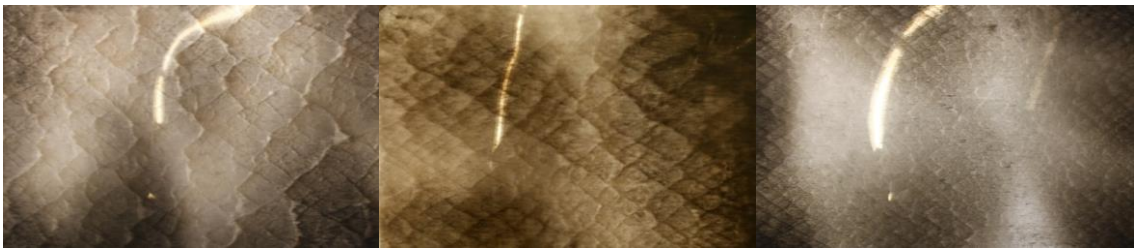
As one of the important dynamic detonation parameters, a wealth of literature can be found on detonation cell size measurement and attempts to develop predictive models. Compared to other combustible mixtures, characteristic detonation cell size values for fuel-$N_2O$ mixtures are relatively scarce. Most of them focused on $H_2/CH_4/NH_3/N_2O$-derived mixtures [2-4].

Recently, a predictive model [5] has been developed based on the Artificial Neural Networks (ANN) approach for a wide range of combustible mixtures and initial conditions using the Konnov mechanism and detonation cell size data summarized at the CalTech Detonation Database [6]. The aim of this study is to validate the wide applicability of this ANN model and compare the existing cell sizes data for $H_2/N_2O$ mixtures and new results measured experimentally for $C_2H_2/N_2O$ and $C_2H_4$-$N_2O$ mixtures using the standard smoked foil technique in a detonation tube facility.

## 2 Experimental Measurement

Cell size measurements using the standard smoked foil technique were obtained from two independent detonation tube facilities: a 26.4 mm-diameter circular detonation tube, with a length of 0.59 m, located at Concordia University, and a tube with a square cross-section of 38.1 mm by 63.5 mm and a length of 2.5-m at Shanghai Jiao Tong University. Average cell sizes of stoichiometric $C_2H_2/N_2O$ mixtures with the initial pressure varying from 4 kPa to 45 kPa were measured. Preliminary results for $C_2H_4/N_2O$ are also obtained. Sample smoked foils for $C_2H_2/N_2O$ mixtures were presented in Fig. 1. Below 10 kPa, the cell size patterns become irregular with sub-structures, increasing the variability in the cell size determination.

**Correspondence to:** georgios.bakalis@mail.concordia.ca 



**(a)** **(b)** **(c)**

**Figure 1:** Sample smoked foils for stoichiometric $C_2H_2/N_2O$ detonation at an initial pressure of 5, 8 and 12 kPa.

## 3 Prediction model based on Artificial Neural Networks

Using the available detonation cell size data from the CalTech Detonation Database [6], together with chemical and thermodynamic parameters as inputs, a Deep Neural Network (DNN) was developed, capable to provide reasonably accurate cell size estimation for a wide variety of gaseous combustible mixtures at different initial conditions with reasonable accuracy, see [5] for the detailed description. The approach was tested for predictive performance with a different and increasing number of features and pre-conditioning of the dataset. In brief, the optimal one is a 3-feature model with 4 hidden layers. The ZND induction length ($\Delta_i$), the detonation Mach number ($M_{CJ}$) and the maximum thermicity ($\dot{\sigma}_{max}$) are determined as the required input features, which are determined from thermodynamic equilibrium and chemical kinetics computations using the CHEMKIN II package [7, 8] with the Konnov's reaction mechanism [9]. Worth noting is that these input parameters with the best performance relate to the description of the detonation reaction zone structure and indirectly to the stability parameter $\chi$ [10], given by the degree of temperature sensitivity in the induction zone $\varepsilon_I$ multiplied by the ratio of induction length $\Delta_I$ to the reaction length $\Delta_R$, which is approximated by the inverse of the maximum thermicity ($1/\dot{\sigma}_{max}$) multiplied by the Chapman-Jouguet (CJ) particle velocity $u'_{CJ}$. Fig. 2 illustrates the structure of this deep neural network model.

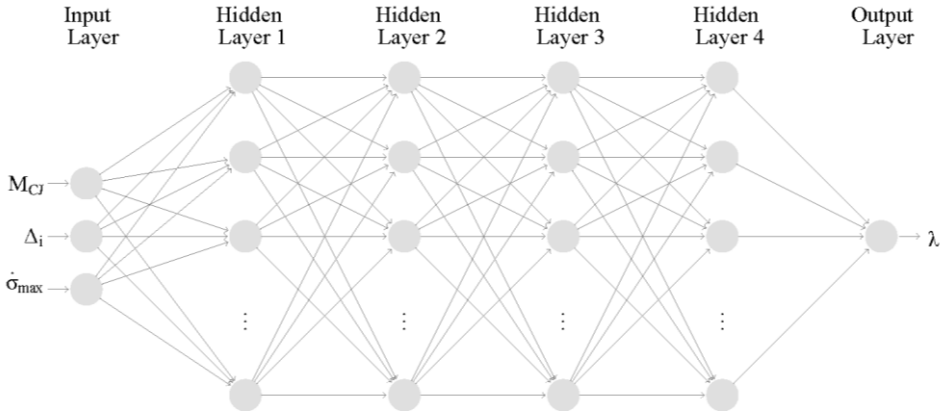
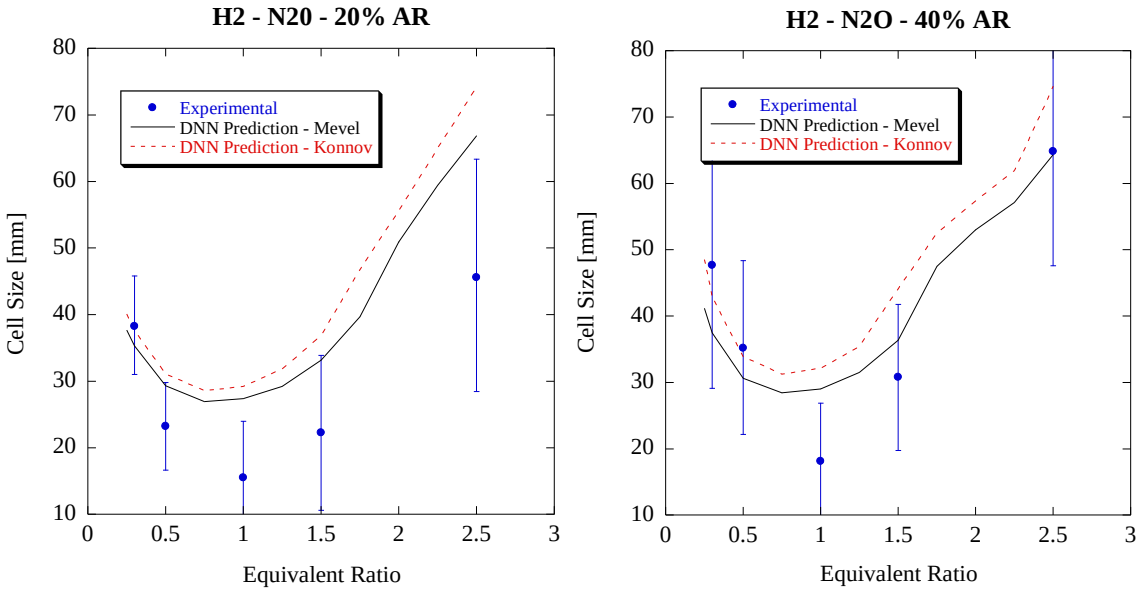



**Figure 2:** Deep Neural Network structure [5]

## 4 Results and discussion

The DNN model is first tested on available experimental data for $H_2/N_2O$ mixtures from [2, 4, 11]. Two mechanisms are chosen, Konnov's [9] and Mével's [4] (version 2012), and the results are given in Figs. 3 and 4.




**Figures 3:** Cell Size prediction using the Konnov and Mével mechanisms compared to the experimental values at different equivalent ratios for $H_2/N_2O$ with a) 20% and b) 40% Ar dilution.

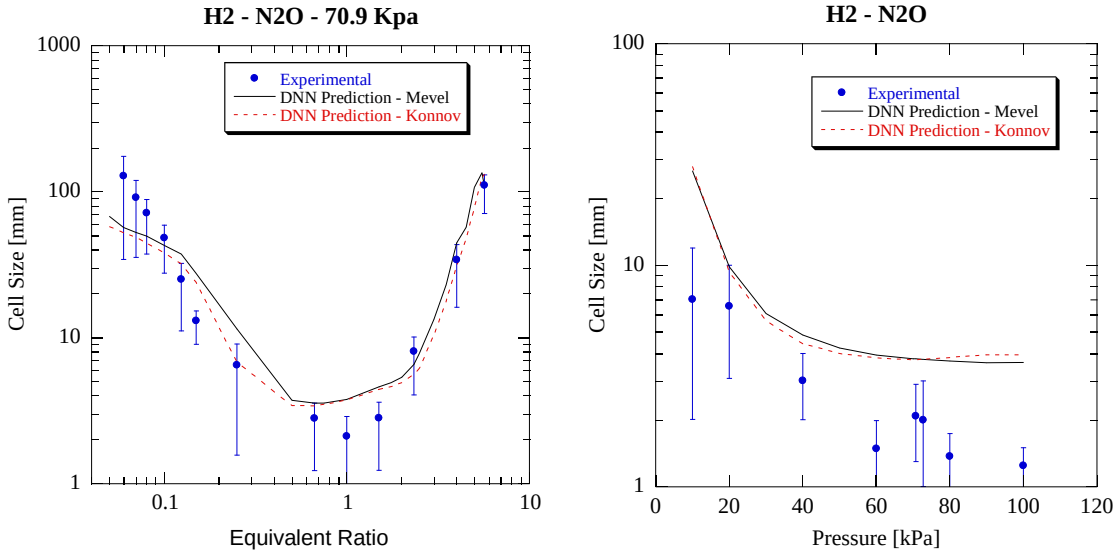



**Figure 4:** Cell Size prediction using the Konnov and Mével mechanisms compared to the experimental values for $H_2/N_2O$ mixtures a) at different equivalent ratios at $p_0$ = 70.9 kPa and b) at different pressures for the stoichiometric condition.

As can be seen, the predictions with both mechanisms are very similar, which is important as the DNN model was created and validated using only the Konnov mechanism. Overall, the model is able to predict well the cell size of the $H_2/N_2O$/Ar mixtures, with better performance for the 20% Ar, despite never having been trained on these mixtures or any mixtures that have $N_2O$ as an oxidizer. For the undiluted $H_2/N_2O$ mixtures (Fig. 4), the prediction accuracy is mixed, with good accuracy for certain pressures ($p_0$ = 20, 40 and 70.9 kPa) and worse but still acceptable for the remaining ones.

The model is then used to predict the cell sizes for the stoichiometric $C_2H_2/N_2O$ mixtures and evaluate the experimental measurements obtained in this study, as shown in Fig. 5. As can be seen in from the results, the model closely agrees with the experimental results from Shanghai university, while varying significantly for the results from Concordia. The smaller measured results at Concordia could be explained by the smaller size of the detonation tube, and thus a bigger influence of the boundary on the detonation propagation as well as the large cell pattern variability at low initial pressure values. The difference could also be attributed to a certain extent to the different geometries of the tubes, which has been shown to affect the cell size [12]. This close agreement between the DNN model and the Shanghai results further validates the model's ability to predict cell sizes of mixtures outside those that were used for its training. It also showcases that it could be used to evaluate experimental cell size measurements when similar measurements are not available for comparison in the literature. To that end, this model was also used for early validation of a second experimental setup at Concordia for the cell size measurements of stoichiometric $C_2H_4$-$N_2O$. At $p_0$ = 30 kPa the model predicted a cell size of 5.73 mm, while the experimental value was 4.56 mm. As this research just started and is ongoing, it is an important indication that this second setup is suitable to accurately measure cell sizes for the given mixture and conditions. Further validations will be made once more experimental results are available. The DNN model thus works as an important, fast, early assessment tool to assess experimental data in mixtures and conditions that have not been explored before. It is expected that this model will become even better as more experimental results become available and are used for its training in the future.

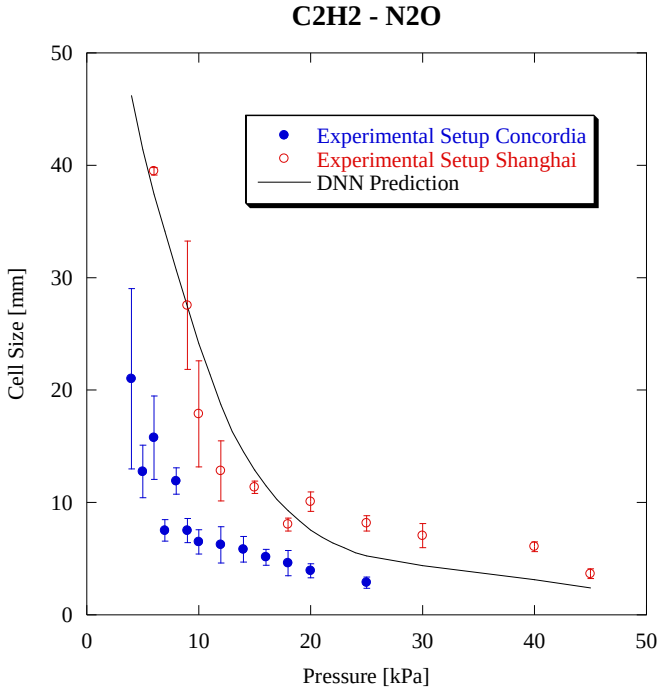



**Figure 5:** Cell size prediction using the Konnov mechanism for stoichiometric $C_2H_2/N_2O$ mixture at different initial pressures, compared to new experimental results obtained from this study.

## 5 Concluding remarks

Detonation cell sizes are measured in this study for the $C_2H_2/N_2O$ and $C_2H_4$-$N_2O$ mixtures and compared with predictions from an artificial neural network model. The model is proven to be a useful

tool to further assess and predict detonations at other uncharacterized initial conditions and blended Hydrogen/Hydrocarbon/Nitrous Oxide mixtures.

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