Nuclear Engineering and Technology xxx (2017) 1–7

Contents lists available at ScienceDirect

Nuclear Engineering and Technology

journal homepage: www.elsevier.com/locate/net

Original Article

Gas detonation cell width prediction model based on support vector regression

Bingxu Hou [a, *], Jiyang Yu [a], Alexander Lelyakin [b], Zhanjie Xu [b], Thomas Jordan [b]

[a] Department of Engineering Physics, Tsinghua University, 100084 Beijing, China
[b] Institute of Nuclear Energy and Technology, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany

ARTICLE INFO

Article history:
Received 28 November 2016
Received in revised form
26 April 2017
Accepted 19 June 2017
Available online xxx

Keywords:
Detonation Cell Width
Hydrogen Safety
Machine Learning
Support Vector Regression

ABSTRACT

Detonation cell width is an important parameter in hydrogen explosion assessments. The experimental data on gas detonation are statistically analyzed to establish a universal method to numerically predict detonation cell widths. It is commonly understood that detonation cell width, λ, is highly correlated with the characteristic reaction zone width, δ. Classical parametric regression methods were widely applied in earlier research to build an explicit semiempirical correlation for the ratio of λ/δ. The obtained correlations formulate the dependency of the ratio λ/δ on a dimensionless effective chemical activation energy and a dimensionless temperature of the gas mixture. In this paper, support vector regression (SVR), which is based on nonparametric machine learning, is applied to achieve functions with better fitness to experimental data and more accurate predictions. Furthermore, a third parameter, dimensionless pressure, is considered as an additional independent variable. It is found that three-parameter SVR can significantly improve the performance of the fitting function. Meanwhile, SVR also provides better adaptability and the model functions can be easily renewed when experimental database is updated or new regression parameters are considered.

© 2017 Korean Nuclear Society, Published by Elsevier Korea LLC. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

1. Introduction

After a severe accident in a nuclear power plant, hydrogen, mainly produced from zirconium–water reaction, can leak into the inner space of the containment. The hazard of hydrogen detonation threatens the integrity of the containment, as in the case of the Fukushima Daiichi nuclear disaster.

When gas detonation takes place, regularly or irregularly distributed cell structures are observed behind the shock wave. The average width of the cells is defined as the detonation cell width, which is represented by λ [1]. The value of λ depends on the initial thermodynamic condition of the flammable gaseous mixture, including the temperature and pressure and the concentrations of the components [2].

λ is commonly used to quantify the detonation risk of flammable gaseous mixtures. For a given gaseous mixture in a given confined volume, the hazard potential caused by detonation may be evaluated with the help of the dimensionless ratio of λ to the characteristic geometric size, noted as L. According to the deflagration-to-detonation transition criterion, which is also known in the field of hydrogen safety research as the λ-criterion, detonation is likely to happen when L/λ is greater than 7 [3]. Therefore, it is of significant importance to reliably predict λ for detonable gases.

To date, there has been no sophisticated theoretical expression to compute λ because of the complexity and uncertainty of the detonation phenomenon. Present solutions to predict the value of λ are all based on empirical or semiempirical correlations established by fitting a large amount of experimental data.

At present, there are two commonly used approaches to estimate λ [4]. One offers simple and direct determination of λ using the initial conditions. In Dorofeev et al [5], a correlation between λ and the initial concentrations of hydrogen and steam, and the initial temperature and pressure is presented. It is clear that such a fit can be used only within the range of the experimental data. Extrapolation of the fitted function beyond the range of measurements does not give reliable values. Another approach is based on an analysis of the correlation of the characteristic reaction zone widths, δ, with λ. The idea that λ and δ can be correlated was first proposed in [6]; such an approach allows estimations of detonation cell sizes for general gas mixtures apart from hydrogen–air–steam mixtures (e.g., hydrocarbon–air mixtures). Quite a few works in the

* Corresponding author.
E-mail address: h.bx@163.com (B. Hou).

http://dx.doi.org/10.1016/j.net.2017.06.014
1738-5733/© 2017 Korean Nuclear Society, Published by Elsevier Korea LLC. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Please cite this article in press as: B. Hou, et al., Gas detonation cell width prediction model based on support vector regression, Nuclear Engineering and Technology (2017), http://dx.doi.org/10.1016/j.net.2017.06.014

UNCORRECTED PROOF

literature [7–9] suggest that two main parameters can influence the stability of the wave and cellular structure. One is the dimensionless effective activation energy, which can be interpreted as a characteristic of the sensitivity of the global reaction time to variations of the postshock temperature caused by changes in the strength of the leading shock. The other is a dimensionless temperature describing the relation between the released chemical energy and the initial thermal energy. In Gavrikov et al [10], mixture composition and initial thermal–dynamic conditions are at first preconditioned into these two parameters. Then, using analytical expressions and the least squares fitting method, a correlation is built between λ/δ and the two dimensionless parameters.

The correlation in Gavrikov et al [10] achieved success in precisely predicting λ within a wide range of thermal conditions for hydrogen–oxidizer mixtures. However, the approach is incapable of predicting λ for hydrocarbon–oxidizer mixtures when the equivalence ratio is larger than 2. Moreover, an attempt to introduce a third parameter to obtain better fitness failed because unphysical oscillations showed up on the regression curves. Because earlier studies suggested that some other parameters could be significant in determining the λ/δ value [1,11], it is necessary to apply better mathematical tools to take more than two parameters into consideration and to improve the precision of the function.

Actually, the aforementioned two approaches are both based on parametric regression. This kind of regression demands an *a priori* assumption of the correlation form, which can be very complicated and difficult to achieve. Meanwhile, parametric regression suffers from weak robustness and poor adaptability performance [12]. When new data points are added and/or additional regression parameters are considered, the regression model can become invalid and needs to be replaced.

To overcome the disadvantages of parametric regression, a nonparametric regression method, support vector regression (SVR), is proposed and discussed in this study. It requires no assumptions about the form of the function, and thus it does not offer an explicit equation but a high-dimensional matrix that describes the relationship among the data points. The fitting process is totally driven by the data itself, leading to better fitness of data and higher stability. The adaptability of the method makes it easier to include new additional data points or new parameters.

The physical idea proposed by Gavrikov et al [10], that λ/δ is a function of dimensionless activation energy and dimensionless temperature, is used and developed in the study. A third parameter, dimensionless pressure, is taken into account to achieve better fitness of data and higher precision.

2. Definitions of parameters

Most of the definitions of the physical parameters involved in this paper utilize the ideas of Gavrikov et al [10]. Some modifications for better regression results are proposed.

2.1. Characteristic reaction zone width

There are several definitions of the characteristic reaction zone width, and in this paper the one expressed by Shepherd [13] is adopted, in which the width is defined as the distance between the leading shock and the location of the maximum rate of temperature rise. The value of the width can be approximately evaluated by the product of the characteristic reaction time, t_{ch}, and the postshock gas velocity, $\overline{D}$:

$$\delta = \overline{D} t_{ch} \tag{1}$$

The original definition of t_{ch} is a period during which the consumption of the limited component is equal to 90% of the total consumption defined by the final equilibrium state. The term "limited component" stands for fuel for lean mixtures or oxidizer for rich mixtures. With such a definition, however, discontinuity occurs for t_{ch} when the equilibration ratio is close to 1, at which point a transition of the reaction process indicator occurs between the fuel and the oxidizer. Therefore, the definition of t_{ch} used in this paper is expressed as an oxidizer consumption equal to 90% of the total consumption defined by the final equilibrium state.

2.2. Dimensionless activation energy

The dimensionless activation energy is defined as $E_a/R/T_{ps}$, where E_a is the effective activation energy, R the gas constant, and T_{ps} the postshock temperature of the gas. The definition of E_a is based on calculations of the characteristic reaction times $t_{ch,1}$ and $t_{ch,2}$ behind shocks with two different traveling speeds D_1 and D_2:

$$\frac{E_a}{R} = \frac{\ln(t_{ch,1}/t_{ch,2})}{1/T(D_1) - 1/T(D_2)} \tag{2}$$

where $T(D_1)$ and $T(D_2)$ are temperatures of the gas behind the shocks with speeds D_1 and D_2, respectively. Meanwhile, these temperatures are also the actual starting temperatures of the chemical reactions. The parameter E_a in Eq. (2) describes the mean sensitivity of the reaction time to the changes in shock strength between D_1 and D_2.

According to an analysis of the reaction conditions in actual multidimensional detonations, as well as prediction accuracy comparisons, Gavrikov et al [10] chose the pair $(1.0D_{cj}, 1.6D_{cj})$ as the values of (D_1, D_2) from the following four candidates:

$$(1.0D_{cj}, 1.6D_{cj}); (1.2D_{cj}, 1.6D_{cj}); (1.0D_{cj}, 1.4Dcj); (1.0D_{cj}, 1.4D_{cj}).$$

where D_{cj} is the Chapman–Jouguet velocity. Two more pairs, $(0.9D_{cj}, 1.6D_{cj})$ and $(0.9D_{cj}, 1.4D_{cj})$, are tested in this study. It is found empirically that, among the six candidate pairs, the pair of $(0.9D_{cj}, 1.6D_{cj})$ always offers the best predictions. According to the classic one-dimensional ZND detonation model, detonation does not occur when D_{cj} is not fully reached. However, to compute activation energy in this model, the speed of $0.9D_{cj}$ in the pair $(0.9D_{cj}, 1.6D_{cj})$ is taken merely as a reference speed. Thus, the calculation of the activation energy is based on the shock strength, regardless of the occurrence of detonation. Therefore, activation energy is computed with $D_1 = 0.9D_{cj}$ and $D_2 = 1.6D_{cj}$, while their mean value $\overline{D} = 1.25D_{cj}$ is used to compute the postshock properties.

2.3. Dimensionless temperature

The ratio of the energy released in reaction to the initial energy of the unignited mixture is expressed as $Q/(C_vT_0)$, where Q is the reaction heat, C_v the constant-volume heat capacity, and T_0 is the initial temperature of the unignited mixture. This ratio describes the relationship between the released chemical energy and the initial thermal energy. However, the value of Q is not defined for the real thermochemistry of a combustible mixture. Meanwhile, a dimensionless temperature T_{vn}/T_0 is related to $Q/(C_vT_0)$ and the variation in the ratio $[Q/(C_vT_0)]/(T_{vn}/T_0)$ is small for most detonable mixtures. It is estimated that, for strong waves of which the Mach number is larger than 2, the variation is within ±25% of an average value of 4.8. Therefore, T_{vn}/T_0 is selected to replace $Q/(C_vT_0)$. T_{vn} is the von Neumann temperature or the temperature of the von Neumann state, which is the maximum extent to which the

UNCORRECTED PROOF

Please cite this article in press as: B. Hou, et al., Gas detonation cell width prediction model based on support vector regression, Nuclear Engineering and Technology (2017), http://dx.doi.org/10.1016/j.net.2017.06.014

دریافت فوری ← متن کامل مقاله

ISIArticles
مرجع مقالات تخصصی ایران

✓ امکان دانلود نسخه تمام متن مقالات انگلیسی
✓ امکان دانلود نسخه ترجمه شده مقالات
✓ پذیرش سفارش ترجمه تخصصی
✓ امکان جستجو در آرشیو جامعی از صدها موضوع و هزاران مقاله
✓ امکان دانلود رایگان ۲ صفحه اول هر مقاله
✓ امکان پرداخت اینترنتی با کلیه کارت های عضو شتاب
✓ دانلود فوری مقاله پس از پرداخت آنلاین
✓ پشتیبانی کامل خرید با بهره مندی از سیستم هوشمند رهگیری سفارشات