



THE IGNITION PARAMETER - A quantification of the risk of ignition

Main author

Niels Bjarne K. Rasmussen
Danish Gas Technology Centre (DGC)
Denmark
NBR@dgc.dk

Co-author

Thomas W. Sødning
Babcock & Wilcox Vølund
Denmark
TWS@volund.dk

1. ABSTRACT

When a mixture of combustible gases is facing or flowing past hot surfaces there is a risk of ignition. But how could this risk be quantified? The present work on quantifying such a risk is presented in this paper including verification of the model. The basic idea of the model of the Ignition Parameter, identified by I_{gn} , is that when I_{gn} is equal to 0.0, no ignition occurs. As I_{gn} increases towards 1.0, the risk of ignition rises to 100%. If I_{gn} is above 1.0, ignition has occurred. The next step is to implement this idea into a useful model.

The basis of the model is empirical data for ignition of combustible gases. For high temperatures it seems that for each of a number of gases the time for ignition can be described by a linear graph in a logarithmic diagram. This leads to a simple Arrhenius expression.

From these data the simple Arrhenius expression for ignition delay time was manipulated to give an expression for the Ignition Parameter I_{gn} .

So

- when I_{gn} is greater than 1, ignition will occur and
- when I_{gn} is less than 1, there is no ignition.

To calculate I_{gn} for any given system it is assumed that the value of I_{gn} can be calculated by solving the general transport equations used in CFD.

A mathematical model was formulated for the Ignition Parameter that takes into account the chemical reaction of chain branching at high temperatures. A different term was formulated for describing the chain termination of reactions, reducing the amount of radicals and the possibility of ignition, especially for colder regions following hot regions. The sum of these terms gives the full source term in CFD modelling of I_{gn} .

In a previous work done at DGC, the code CHEMKIN was used to calculate the autoignition temperature for natural gas at different gas mixtures and residence times. In this model, hundreds of species and thousands of chemical reactions were included to give the best possible result. The results obtained by CHEMKIN were used as empirical data for the Ignition Parameter to calculate the empirical constants needed for the model.

To find experimental data of ignition for mixtures of natural gas and air and to test the model of Ignition Parameter an experimental setup was established

A pellet was slowly heated electrically until ignition of a steady state flow of a mixture of gas and air passing the pellet. The temperature of the pellet at ignition was found.

Five different experiments with steel pellet and different gas/air mixtures were established. The data from these experiments were compared to the CFD calculation of the same cases.

The present work has shown that by using this simple one-equation model a very good representation of the ignition time has been reached. Furthermore, using this model of Ignition Parameter in CFD modelling we have found that the model calculates the ignition temperature of an actual test case within an error of 0-50K on the safe side. This was found for the above test cases, in which the heated test object was used to ignite a mixture of natural gas and air.

This model for ignition could be implemented and applied for different purposes. In the use of CFD with combustion modelling, ignition of the mixture is a critical problem. Using this ignition model could give a measure of the time and location for ignition. When the Ignition Parameter in the model exceeds 1.0, ignition could be initiated at that point in the model. This would give a fairly good model for ignition in the combustion modelling with CFD.

Furthermore, the model could be used in CFD-modelling of safety issues. When new standards are to be found for explosive and combustible gases this model could be used for test cases to predict the risk of ignition in each case.

The model of the Ignition Parameter could be used in all cases where the knowledge of the risk of ignition of a gas/air mixture is wanted. In the present case the model is used for natural gas and air mixtures. However, any other combustible gas could be modelled in the same way by establishing the empirical constants related to the model.

The model of the Ignition Parameter is a novel model, which gives very good results and may be a great help in predicting risks of ignition of combustible gases close to hot surfaces.

From the results shown in this paper we conclude that it is possible to calculate and predict the risk of autoignition for natural gas near a heated surface in relation to a given natural gas mixture within the explosion limits.

Keywords: ignition parameter, quantification, risk of ignition, ignition time, delay, CFD, CHEMKIN

CONTENTS

1. Abstract	2
2. The idea of the Ignition Parameter	5
3. Empirical data on ignition	5
4. Arrhenius expressions based on empirical data	7
5. Equation of Balance and Source and Sink of the Ignition Parameter.....	9
5.1. Equation of balance.....	9
5.2. The source term at high temperatures	10
5.3. The sink term for Ignition Parameter	11
5.4. Calculation of the constants	12
5.5. The source term of the Ignition Parameter in CFD modelling	13
6. Experimental setup with hot pellet in gas flow	14
7. CFD modelling and comparison	15
8. Implementation and application of the model.....	17
9. Conclusions	18
10. Acknowledgment	19
11. References	19

2. THE IDEA OF THE IGNITION PARAMETER

When a mixture of combustible gases is facing or flowing past hot surfaces there is a risk of ignition. But how could this risk be quantified? The present work on quantifying such a risk is presented in this paper including verification of the model. The basic idea of the model of the Ignition Parameter, identified by I_{gn} , is that when I_{gn} is equal to 0.0, no ignition occurs. As I_{gn} increases towards 1.0, the risk of ignition rises to 100%. If I_{gn} is above 1.0, ignition has occurred. The next step is to implement this idea into a useful model /3/.

3. EMPIRICAL DATA ON IGNITION

The basis of the model is empirical data for ignition of combustible gases. Figure 1 shows an example of such data.

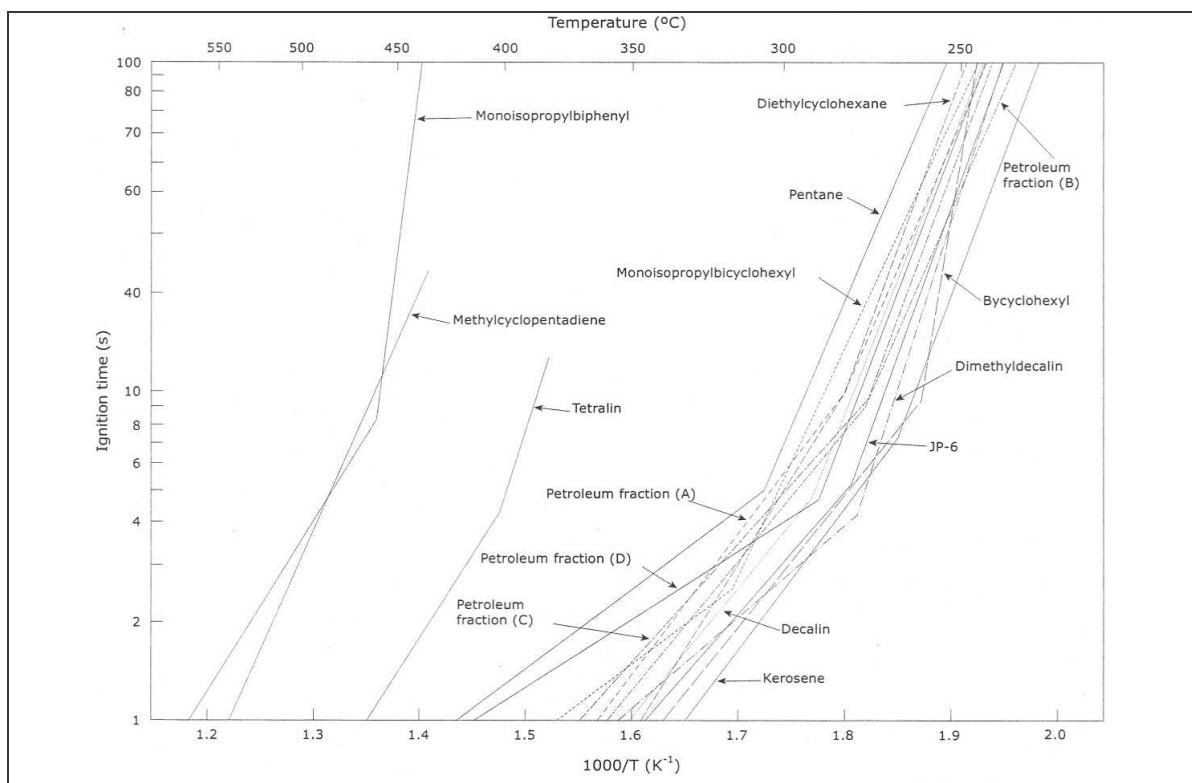


Figure 1 Ignition times for a number of gases measured by Bureau of Mines (Babrauskas, 2003)

For high temperatures it seems that for each of the gases the time for ignition can be described by a linear graph in a logarithmic diagram. This leads to a simple Arrhenius expression where the following relation between ignition time and temperature can be used.

$$\ln \tau_{ign} = \left(\frac{E}{R} \right) \frac{1}{T} + a \quad (1)$$

Here a is an experimental constant, E is the activation energy [J/mol], R is the ideal gas law constant [J/molK], T is the autoignition temperature [K], and τ_{ign} is the time to ignition [s]. If a simple Arrhenius expression for global kinetics would be sufficient for any gas, results for any particular gas would fall along a single straight line.

As can be seen in Figure 1, most gases show lines with two slopes: one at higher temperature and one at lower temperature regime. Interestingly, given the large number of reactions taking place in real gases, the curves are all composed of two straight lines, rather than being complex curves.

Furthermore, if the time scale were extended further it might be the case that an asymptotic vertical line would occur for each graph. This means that below a certain temperature no ignition will occur, no matter the exposure time. That would be a vertical line in the diagram.

In a previous work done at DGC, the code CHEMKIN was used to calculate the autoignition temperature for natural gas at different gas mixtures and residence times. The results from these calculations are shown in Figure 2. In this model, hundreds of species and thousands of chemical reactions were included to give the best possible result.

While Figure 1 shows the ignition time for a fixed mixture of fuel and air for different fuels, Figure 2 shows the relation between temperature and ignition time for a wide range of mixtures of natural gas and air.

The AIT, "AutoIgnition Temperature", is the lowest temperature for which autoignition will occur with the given mixture of gases and for a very long residence time (600-900 sec).

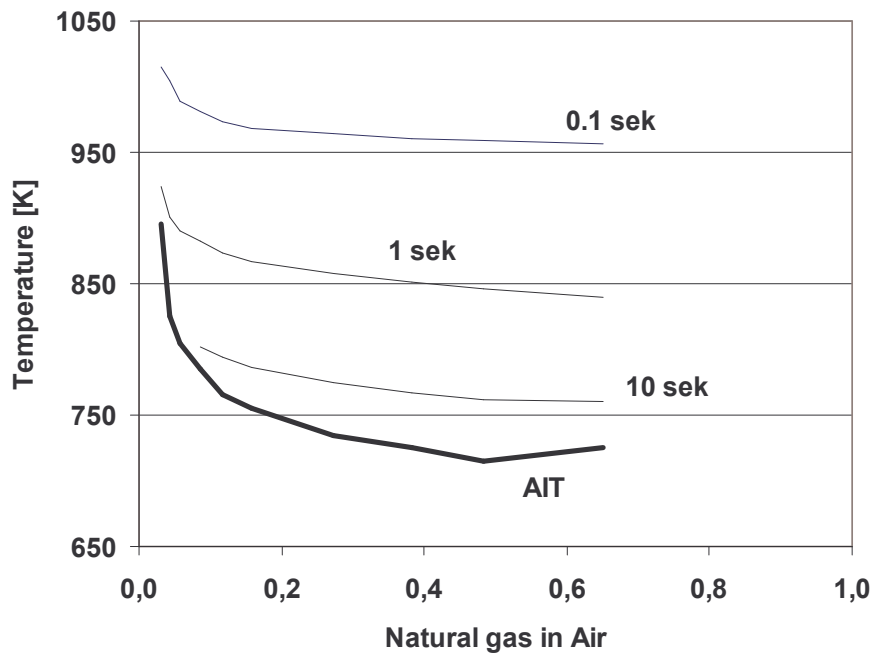


Figure 2 CHEMKIN calculated correlation between temperature and ignition time for natural gas in air

4. ARRHENIUS EXPRESSIONS BASED ON EMPIRICAL DATA

For a system with a high temperature and a given gas mixture it was shown in the previous section that if simple Arrhenius kinetics is assumed, then equation (1) can apply and then the following equation can be used:

$$\ln \tau_{ign} = a_1 + \frac{T_{act}}{T} \quad (2)$$

Here E/R (from equation (1)) is called the activation temperature T_{act} . This can be rewritten into the following equation:

$$\text{constant} = \tau_{ign} \cdot \exp\left(\frac{-T_{act}}{T}\right) [-] \quad (3)$$

where τ_{ign} is the time delay before ignition, also known as the ignition time. T_{act} is a constant found experimentally for a given gas mixture. If we also take into account the concentration of a combustible gas [fuel] mixed with air [air] we arrive at:

$$\text{constant} = \tau_{ign} \cdot \exp\left(\frac{-T_{act}}{T}\right) [\text{fuel}]^C [\text{air}]^D [-] \quad (4)$$

and by dividing by the constant we get:

$$1 = \tau_{ign} \cdot A \cdot \exp\left(\frac{-T_{act}}{T}\right) [fuel]^C [air]^D \quad [-] \quad (5)$$

At this point we introduce the Ignition Parameter I_{gn} . If τ instead is viewed as the residence time with constant conditions on the right side of the equation, the left side can be viewed as an Ignition Parameter I_{gn} :

$$I_{gn} = \tau \cdot A \cdot \exp\left(\frac{-T_{act}}{T}\right) [fuel]^C [air]^D \quad [-] \quad (6)$$

valid for high temperatures.

So

- when I_{gn} is greater than 1, ignition will occur and
- when I_{gn} is less than 1, there is no ignition.

This is illustrated in Figure 3.

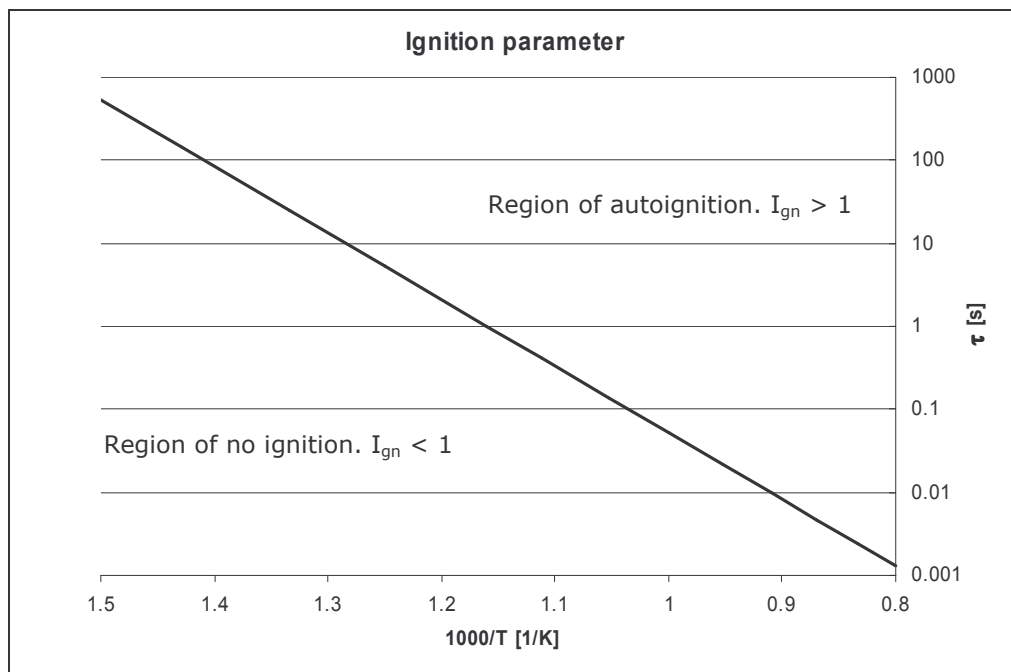


Figure 3 Logarithm of time delay before ignition as a function of the temperature, $I_{gn}=1$. The regions for no ignition and autoignition are also shown.

5. EQUATION OF BALANCE AND SOURCE AND SINK OF THE IGNITION PARAMETER

5.1. Equation of balance

To calculate I_{gn} for any given system it is assumed that the value of I_{gn} can be calculated by solving the general transport equations used in CFD. If we introduce a general variable, ϕ , then the conservative form of all fluid flow equations can be written in the following way:

$$\frac{\partial(\rho \cdot \phi)}{\partial t} + \frac{\partial}{\partial x_i}(\rho \cdot \phi \cdot u_i) = \frac{\partial}{\partial x_i} \left(\Gamma \frac{\partial \phi}{\partial x_i} \right) + S_\phi \quad (7)$$

where ρ is the density, t is the time, Γ is the diffusion coefficient, S is the source term for the variable ϕ , and u_i and x_i are the velocity and the distance, respectively, in the i -direction. In words, the general transport equations can be described as:

Rate of increase of ϕ in fluid element	+	Net rate of flow of ϕ out of fluid element	=	Rate of increase of ϕ due to diffusion	+	Rate of increase of ϕ due to source
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The Equation (7) is the transport equation for property ϕ . It highlights the various transport processes: the rate of change term and the convection term on the left side and diffusive term and the source term on the right side. In order to bring out the common features in the general equation we have hidden the terms not shared between the equations in the source term. So to solve I_{gn} we have to replace ϕ with I_{gn} as shown in equation (8).

$$\frac{\partial(\rho \cdot I_{gn})}{\partial t} + \frac{\partial}{\partial x_i}(\rho \cdot I_{gn} \cdot u_i) = \frac{\partial}{\partial x_i} \left(\Gamma_I \frac{\partial I_{gn}}{\partial x_i} \right) + S_{ign} \text{ [kg/m}^3\text{s]} \quad (8)$$

Equation (8) is the full balance equation for the Ignition Parameter I_{gn} .

The next problem is to find the source term S_{ign} .

5.2. The source term at high temperatures

First, we consider a steady state condition and assume a case where diffusion can be neglected. Equation (8) is then reduced to:

$$\frac{\partial}{\partial x_i} (\rho \cdot I_{gn} \cdot u_i) = S_{ign} \quad [\text{kg/m}^3\text{s}] \quad (9)$$

Using the continuity equation:

$$\frac{\partial}{\partial x_i} (\rho \cdot u_i) = 0 \quad [\text{kg/m}^3\text{s}] \quad (10)$$

we reduce equation (9) to:

$$\rho \cdot u_i \frac{\partial I_{gn}}{\partial x_i} = S_{ign} \quad [\text{kg/m}^3\text{s}] \quad (11)$$

Equation (6) for high temperatures can be reformulated to:

$$I_{gn} = \tau \cdot f(T, fuel, air) \quad [-] \quad (12)$$

where τ is the residence time and $f(T, fuel, air)$ is the Arrhenius function of the temperature and the concentration of fuel and air. Using equation (12) in (11) we get:

$$\rho \cdot u_i \cdot \left(\tau \frac{\partial f(T, fuel, air)}{\partial x_i} + f(T, fuel, air) \frac{\partial \tau}{\partial x_i} \right) = S_{ign} \quad [\text{kg/m}^3\text{s}] \quad (13)$$

If, furthermore, we assume that the temperature and concentration of the species are constant for our system of interest then $f(T, fuel, air)$ is constant and we get:

$$\rho \cdot u_i \cdot f(T, fuel, air) \frac{\partial \tau}{\partial x_i} = S_{ign} \quad [\text{kg/m}^3\text{s}] \quad (14)$$

At this point the following approximation is made:

$$\frac{\partial \tau}{\partial x_i} = u_i^{-1} \quad [\text{s/m}] \quad (15)$$

and including this into (14) the following is obtained:

$$S_{ign} = \rho \cdot f(T, fuel, air) \text{ [kg/m}^3\text{s]} \quad (16)$$

With the above assumptions we now have a source term for the Ignition Parameter, I_{gn} , described by equation (16).

The equation (16) was deduced for 1-D constant property conditions. However, it is assumed to be valid in 3-D real conditions.

We have now formulated a mathematical model for the Ignition Parameter that takes into account the chemical reaction of chain branching at high temperatures. We also need a term for describing the chain termination of reactions, reducing the amount of radicals and the possibility of ignition, especially for colder regions following hot regions.

5.3. The sink term for Ignition Parameter

Imagine a flammable gas mixture flowing in an infinitely long pipe, which in turn is heated and cooled along the length. If the Ignition Parameter is only calculated by the source term of equation (16), the model will predict that the gas mixture will eventually ignite. In a real situation the cooling of the gas mixture will terminate some of the chemical reactions and prolong the time to ignition or prevent the ignition.

To take into account the effect of cooling a negative source term is introduced:

$$S_{ink} = -B \cdot I_{gn} \text{ [kg/m}^3\text{]} \quad (17)$$

B is a constant and this sink term will reduce the value of I_{gn} in areas where the gas mixture is cooled. The logic behind equation (17) is that radicals combine and thereby reduce the risk of ignition. This combination of radicals is assumed to be independent of temperature and solely dependent on the concentration of radicals. The Ignition Parameter I_{gn} is a measure of the radicals concentration and hence equation (17).

The new expression for the combined source and sink term is then

$$S_{ign} = \rho \cdot f(T, fuel, air) - B \cdot I_{gn} \text{ [kg/m}^3\text{s]} \quad (18)$$

replacing equation (16) for high as well as low temperatures.

5.4. Calculation of the constants

By combining the equations (12) and (16) the following equation is obtained

$$I_{gn} = \tau \frac{S_{ign}}{\rho} [-] \quad (19)$$

which is assumed to be valid with the new source term of equation (18). The Arrhenius expression for the Ignition Parameter can then be changed to:

$$I_{gn} = \tau \left[f(T, fuel, air) - \frac{B}{\rho} \cdot I_{gn} \right] [-] \quad (20)$$

replacing equation (12). In the case of ignition $\tau = \tau_{ign}$ and $I_{gn} = 1$ and we get

$$1 = \tau_{ign} \left[f(T, fuel, air) - \frac{B}{\rho} \right] [-] \quad (21)$$

replacing equation (5). If we assume that the gas mixture is an ideal gas, then the density can be replaced and we get the following equation:

$$\frac{1}{\tau_{ign}} = f(T, fuel, air) - B \frac{R \cdot T}{M \cdot p} [\text{kg/m}^3\text{s}] \quad (22)$$

where R is the ideal gas constant, T is the temperature, M is the molar mass of the gas mixture and p is the pressure. Unfolding the function $f(T, fuel, air)$ we get equation (23).

$$\frac{1}{\tau_{ign}} = A \cdot \exp\left(\frac{-T_{act}}{T}\right) [fuel]^c [air]^d - B \frac{R \cdot T}{M \cdot p} [1/\text{s}] \quad (23)$$

The interpretation of equation (23) is as follows. The first term on the right side is due to chain branching and radicals production while the second term is due to chain termination and decay of radicals. For very high temperatures, τ_{ign} is very small and the second term (decay) may be neglected. For low autoignition temperatures with very high residence time, τ_{ign} is very large and decay and production of radicals are equal (left side = 0). This is related to Figure 1. For high temperatures all graphs of this figure have straight lines. At certain low temperatures all graphs approach asymptotically a separate vertical line with infinite ignition time.

The constants A , B , C , D and T_{act} are empirical. With equation (23) together with empirical data for a given gas mixture and the ignition time it is possible to calculate the empirical constants.

The values for A , T_{act} , C and D are found at high temperatures and small residence time, thereby neglecting the second term. The value of B is found at the tabulated autoignition temperature for the gas mixture, i.e. when the ignition time is infinite.

The final expression for the Ignition Parameter source term is equation (18) and how it is used in CFD is shown in the following section. The equation (8) is solved by CFD.

5.5. The source term of the Ignition Parameter in CFD modelling

In the CFD programme STAR-CD it is possible to introduce new scalars in the subroutine and to enable the user to specify source terms (per unit volume) for scalars in the following linearized form:

$$S = S_1 - S_2 I \quad [\text{kg}/\text{m}^3\text{s}] \quad (24)$$

To model the Ignition Parameter the source term parameters for the scalar I_{gn} are:

$$S_1 = \rho \cdot A \cdot \exp\left(\frac{-T_{act}}{T}\right) [\text{fuel}]^C [\text{air}]^D \quad [\text{kg}/\text{m}^3\text{s}] \quad (25)$$

and

$$S_2 = B \quad [\text{kg}/\text{m}^3\text{s}] \quad (26)$$

The results obtained by CHEMKIN (Figure 2) were used as empirical data for the Ignition Parameter to calculate the empirical constants A , B , C , D and T_{act} by data fitting. The values of the empirical constants were used in equation (23) and the following figure was obtained.

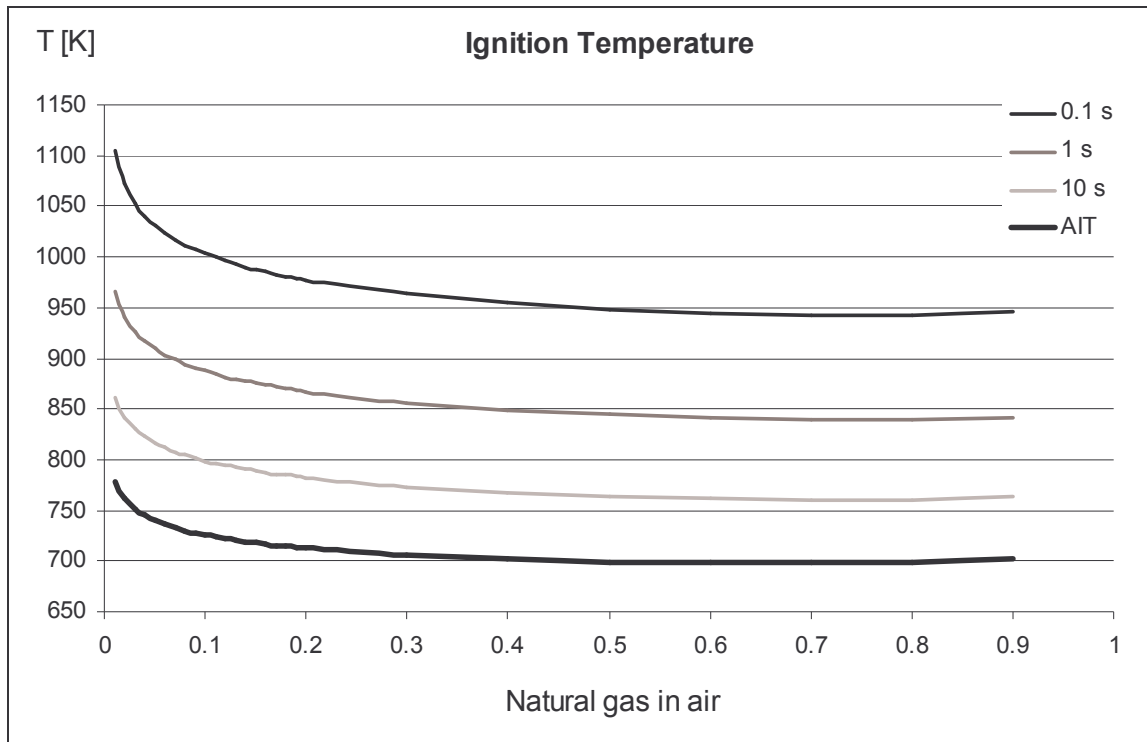


Figure 4 Calculated correlation between temperature and ignition time for natural gas in air by the use of the one equation model of equation (23)

The first thing we notice when comparing Figure 4 with Figure 2 is that the trend of the curves is the same. Secondly, the lowest autoignition temperatures for all the residence times are at approximately the same mixture range. Figure 4 also assumes that the Ignition Parameter is valid at natural gas in air mixtures lower than 4% and greater than 65% to be compared to Figure 2. This is a conservative approach and is on the safe side when performing risk analyses.

With the model for the Ignition Parameter formulated and the empirical constants found it is now possible to model the autoignition phenomenon for gas mixtures of natural gas and air.

6. EXPERIMENTAL SETUP WITH HOT PELLET IN GAS FLOW

To find experimental data of ignition for mixtures of natural gas and air and to test the model of Ignition Parameter an experimental setup was established

An overview of the test rig with the test object is shown in Figure 5. The height of the test rig is about 2 m and the test object has the size of 16 cm.

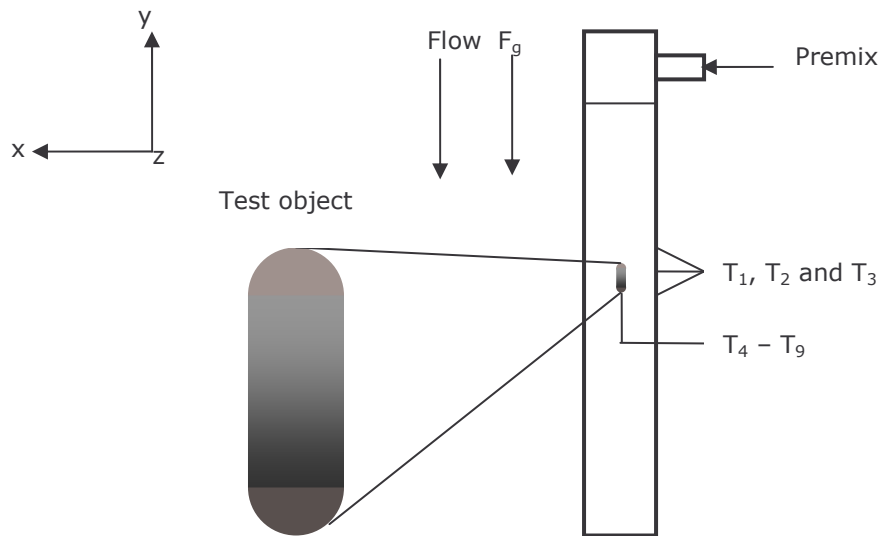


Figure 5 Overview of the geometry of the test rig

The flow of premixed gas/air was from top and down. The pellet was slowly heated electrically until ignition of the mixture. The temperature of the pellet at ignition was found.

Five different experiments with steel pellet and different gas/air mixtures were established. The data from these experiments were compared to the CFD calculation of the same cases.

7. CFD MODELLING AND COMPARISON

To model the flow and the temperature field in the test rig and around the test object the programme STAR-CD v3.26 was used.

DGC has developed an in-house radiation model known as The Composite Radiosity and Gap (CRG) model of thermal radiation, which is fast and better than the built-in radiation models in STAR-CD. The built-in turbulence model in STAR-CD has been modified and improved by DGC.

To model the Ignition Parameter the model formulated in Section 4 with the constants for natural gas from Section 5 was implemented in STAR-CD as to model the flow, radiation and ignition of the test cases.

The first results obtained by the CFD modelling for the five test cases showed good results. The maximum Ignition Parameter was by a factor of 1.0 to 2.3 more than

expected, as shown in Table 1. Maximum Ignition Parameter I_{gn} would be expected to be 1.0 at autoignition.

To estimate how much the CFD model is on the conservative side the temperatures for the test object were reduced so that the maximum Ignition Parameter (max. I_{gn}) was approximately 1.0. In Table 1 dT is the necessary reduction of the temperatures in the CFD modelling compared to the test case to reach a max. calculated Ignition Parameter of 1.0 along the heated test object.

The present work has shown that by using this simple one-equation model a very good representation of the ignition time (Figure 2) was reached. Furthermore, using this model of Ignition Parameter in CFD modelling we have found that the model calculates the ignition temperature of an actual test case within an error of 0-50K on the safe side. This was found for the above test cases, in which the heated test object was used to ignite a mixture of natural gas and air.

Table 1 The CFD-calculated Ignition Parameter for the test object at autoignition conditions in the test rig

Test	First results				With reduced temperatures	
	Natural gas in air [% _{vol}]	Residence time [s]	Test object mean temp. [K]	Max. I_{gn} [-]	Max. I_{gn} [-]	dT [K]
0	11.54	0.86	1030	2.254	1.017	47
1	8.67	0.87	1023	1.595	1.006	27
2	6.15	0.87	1022	1.193	1.001	10
3	5.93	1.04	1018	0.964	1.015	-2
4	8.86	1.01	1007	1.028	1.002	2

8. IMPLEMENTATION AND APPLICATION OF THE MODEL

This model for ignition could be implemented and applied for different purposes. In the use of CFD with combustion modelling, ignition of the mixture is a critical problem. Using this ignition model could give a measure of the time and location for ignition. When the Ignition Parameter in the model exceeds 1.0, ignition could be initiated at that point in the model. This would give a fairly good model for ignition in the combustion modelling with CFD.

Furthermore, the model could be used in CFD-modelling of safety issues. When new standards are to be found for explosive and combustible gases this model could be used for test cases to predict the risk of ignition in each case.

The model of the Ignition Parameter could be used in all cases where the knowledge of the risk of ignition of a gas/air mixture is wanted. In the present case the model is used for natural gas and air mixtures. However, any other combustible gas could be modelled in the same way by establishing the empirical constants related to the model.

9. CONCLUSIONS

The model of the Ignition Parameter is a novel model, which gives very good results and may be a great help in predicting risks of ignition of combustible gases close to hot surfaces.

From the results shown in this paper we conclude that it is possible to calculate and predict the risk of autoignition for natural gas near a heated surface in relation to a given natural gas mixture within the explosion limits.

From the present work it can be seen that starting with the CHEMKIN modelling giving the ignition delay time (results of Figure 2), then through the one-equation model, (equation (23)), giving the results of Figure 4, and finally using equations (24)-(26) in CFD modelling of an actual test case we get results with errors of the ignition temperature of only 0-50K (on the safe side). These errors include all the possible errors from the CHEMKIN modelling, from the derived one-equation model, from the experimental data and finally from the CFD modelling of the experimental setup.

That is a fairly good result.

10. ACKNOWLEDGMENT

This work /1/, /2/ has been supported by the Danish gas companies (The Executive Technical Committee) who are greatly acknowledged.

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