THE IGNITION PARAMETER -
A quantification of the probability of ignition
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Topic: Modelling of fundamental processes

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Abstract

When a mixture of combustible gases is facing or flowing past hot surfaces there is a probability of ignition. But how can this probability be quantified? The work on quantifying such a probability of ignition is presented in this paper including verification of the model.

The basic idea of this model of the Ignition Parameter, identified by I_{gn}, is that when $I_{gn} \geq 1$ ignition will occur, and when $I_{gn} < 1$ no ignition will occur. The model is based on empirical data for ignition of combustible gases. For high temperatures it seems that for each of the gases the time delay for ignition can be described by a linear graph in a logarithmic diagram. This leads to a simple Arrhenius expression.

To calculate the Ignition Parameter I_{gn} by CFD modelling the following equation is assumed to be valid:

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

This equation is the transport equation for I_{gn}. 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. The expression for the combined source and sink term is

$$S_{ign} = \rho \cdot A \cdot \exp\left(\frac{-E}{RT}\right)[fuel]^C[air]^D - B \cdot I_{gn} \text{ [kg/m}^3\text{s]}$$

This equation is related to the ignition time delay and the Arrhenius expression is recognized.

The code CHEMKIN was used to calculate the autoignition temperature for natural gas at different gas mixtures and residence times. The results were used as empirical data for the Ignition Parameter to calculate the empirical constants A, B, C, D and E by data fitting. The interpretation of the second equation 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.

The model was compared to experimental data. A steel pellet was slowly heated electrically until ignition of a steady state flow of a premix of gas and air passing the pellet. The temperature of the pellet at ignition was found. The data from these experiments were compared to the CFD calculations of the same cases. Ideally, the results for I_{gn} should end at 1.0 as maximum in the volume in each case.

We have found that the model calculates the ignition temperature of actual test cases within deviations of only 0-50K and on the lower side. These deviations include all the possible uncertainties from the CHEMKIN modelling, from the derived one-equation model, from the experimental data and, finally, from the CFD modelling of the experimental setup. The model of the Ignition Parameter is a novel model, which gives very good results and may be a great help in predicting probabilities of ignition of combustible gases close to hot surfaces.

Keywords: ignition parameter, probability of ignition, ignition time, delay, CFD, CHEMKIN

Introduction

When a mixture of combustible gases is facing or flowing past hot surfaces there is a probability of ignition. But how can this probability be quantified? The work on quantifying such a probability of ignition is presented in this paper including verification of the model. The basic idea of this model of the Ignition Parameter, identified by I_{gn}, is that when

- $I_{gn} \geq 1$ ignition will occur
- $I_{gn} < 1$ no ignition will occur

As I_{gn} increases towards 1.0 at any point throughout the volume of interest, the risk of ignition rises to 100%. If I_{gn} is above 1.0, ignition has occurred. If I_{gn} keeps below 1.0, no ignition occurs in the volume. The next step is to implement this idea into a useful model /3/.

Empirical data on ignition

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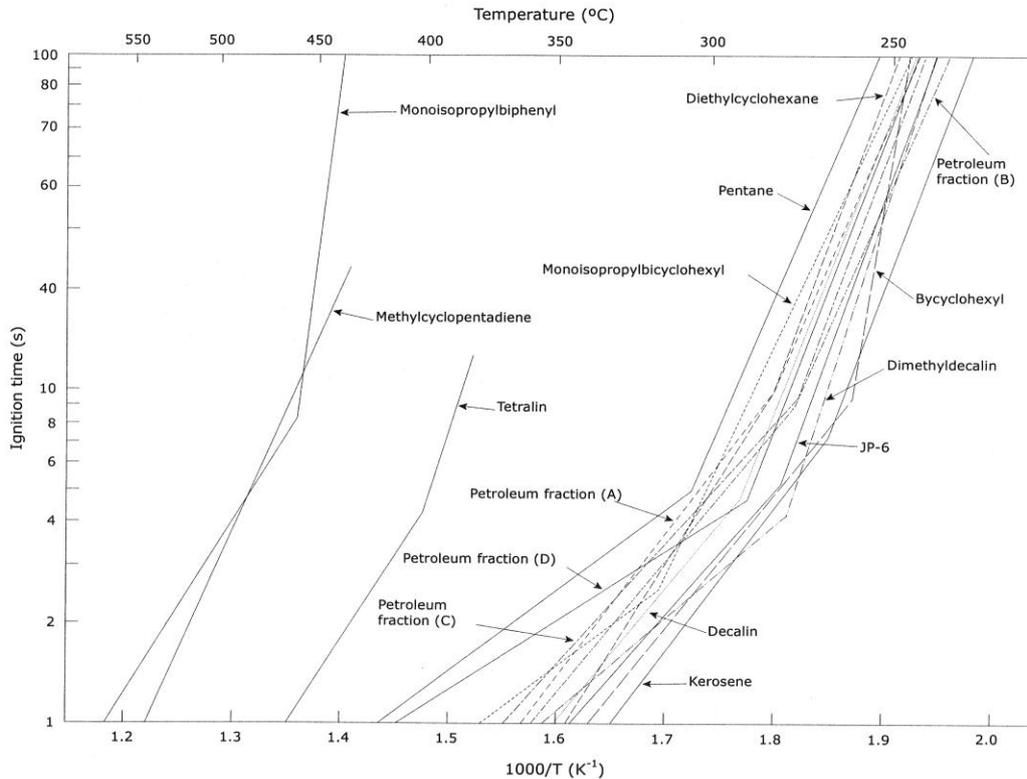

Figure 1 Ignition times for a number of gases measured by Bureau of Mines (Babrauskas, 2003)

For high temperatures it seems that for each of the gases the time delay 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 delay and temperature can be used:

$$\ln \tau_{ign} = \frac{E}{RT} + a \Leftrightarrow \frac{1}{\tau_{ign}} = A \cdot \exp\left(\frac{-E}{RT}\right) \qquad (1)$$

- a and A are experimental constants
- E is the activation energy [J/mol]
- R is the ideal gas law constant [J/molK]
- T is the temperature [K]
- τ_{ign} is the ignition time delay [s]

As found 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.

If we also take into account the concentration of a combustible gas [fuel] mixed with air [air], equation (1) can be rewritten and expanded to the following in which it is assumed that the dependency of concentrations can be described by the exponents C and D:

$$1 = \tau_{ign} \cdot A \cdot \exp\left(\frac{-E}{RT}\right)[fuel]^{C}[air]^{D} \text{ [-]} \qquad (2)$$

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

$$I_{gn} = \tau \cdot A \cdot \exp\left(\frac{-E}{RT}\right)[fuel]^{C}[air]^{D} \text{ [-]} \qquad (3)$$

valid for high temperatures only. So

- when I_{gn} is greater than 1, corresponding to $\tau > \tau_{ign}$, ignition will occur and
- when I_{gn} is less than 1, corresponding to $\tau < \tau_{ign}$, there is no ignition.

CHEMKIN calculations

The code CHEMKIN was used to calculate the ignition 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.

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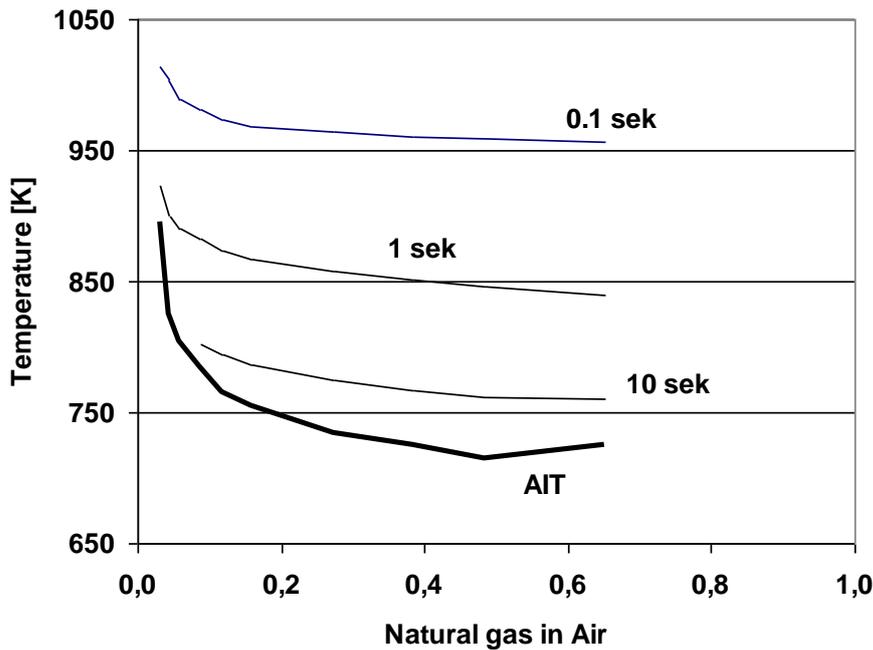
Figure 2   CHEMKIN calculated correlation between temperature and ignition time for natural gas in air

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.

A vertical line in Figure 2 could be implemented as a graph for natural gas in Figure 1, the AIT being the mentioned vertical line below which temperature no ignition would occur.

Equations for the Ignition Parameter

To calculate the Ignition Parameter I_{gn} by CFD modelling the following equation is assumed to be valid, i.e. it is assumed that I_{gn} can be solved like any other variable as temperature or concentrations.

$$\frac{\partial(\rho \cdot I_{gn})}{\partial t} + \frac{\partial}{\partial x_i}(\rho \cdot I_{gn} \cdot u_i) = \frac{\partial}{\partial x_i}\left(\Gamma_I \frac{\partial I_{gn}}{\partial x_i}\right) + S_{ign} \text{ [kg/m}^3\text{s]} \qquad (4)$$

- ρ is the density
- t is the time
- Γ is the diffusion coefficient
- S_{ign} is the source term for the variable I_{gn}
- u_i is the velocity
- x_i is the distance in the i-direction

The equation (4) is the transport equation for I_{gn}. 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.

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

The source term at high temperatures

First, we consider a steady state condition and assume a case where diffusion can be neglected. Equation (4) is then reduced to:

$$\frac{\partial}{\partial x_i}\left(\rho \cdot I_{gn} \cdot u_i\right) = S_{ign} \ \text{[kg/m}^3\text{s]} \tag{5}$$

Using the continuity equation:

$$\frac{\partial}{\partial x_i}\left(\rho \cdot u_i\right) = 0 \ \text{[kg/m}^3\text{s]} \tag{6}$$

we reduce equation (5) to:

$$\rho \cdot u_i \frac{\partial I_{gn}}{\partial x_i} = S_{ign} \ \text{[kg/m}^3\text{s]} \tag{7}$$

Equation (3) for high temperatures can be reformulated to:

$$I_{gn} = \tau \cdot f \ \text{[-]} \tag{8}$$

where τ is the residence time and f is the Arrhenius function of the temperature and the concentration of fuel and air. Using equation (8) in (7) we get:

$$\rho \cdot u_i \cdot \left(\tau \frac{\partial f}{\partial x_i} + f \frac{\partial \tau}{\partial x_i}\right) = S_{ign} \ \text{[kg/m}^3\text{s]} \tag{9}$$

If, furthermore, we assume that the temperature and concentration of the species are constant for our present system then f is constant and we get:

$$\rho \cdot u_i \cdot f \frac{\partial \tau}{\partial x_i} = S_{ign} \ \text{[kg/m}^3\text{s]} \tag{10}$$

At this point the following approximation is made (related to 1-D conditions):

$$\frac{\partial \tau}{\partial x_i} = u_i^{-1} \ \text{[s/m]} \tag{11}$$

and including this into (10) the following is obtained:

$$S_{ign} = \rho \cdot f \ \text{[kg/m}^3\text{s]} \tag{12}$$

With the above assumptions we now have a source term for the Ignition Parameter, I_{gn}, described by equation (12) only valid for high temperatures.

The equation (12) 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.

The sink term for the 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 (12), 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:

$$S_{ink} = -B \cdot I_{gn} \text{ [kg/m}^3\text{]}$$ (13)

B is a positive constant and this sink term will reduce the value of I_{gn} in areas where the gas mixture is cooled. The logic behind equation (13) 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 (13).

Combined source and sink term for all temperatures

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

$$S_{ign} = \rho \cdot f - B \cdot I_{gn} \text{ [kg/m}^3\text{s]}$$ (14)

replacing equation (12) for high as well as low temperatures. By unfolding the expression for the combined source and sink term (eq. 14) the following emerges:

$$S_{ign} = \rho \cdot A \cdot \exp\left(\frac{-E}{RT}\right)[fuel]^C[air]^D - B \cdot I_{gn} \text{ [kg/m}^3\text{s]}$$ (15)

By the use of the above equations and assuming ideal gases it can be shown that the equation (15) is related to the ignition time delay of Figure 1 in the following way:

$$\frac{1}{\tau_{ign}} = A \cdot \exp\left(\frac{-E}{RT}\right)[fuel]^C[air]^D - B \frac{R \cdot T}{M \cdot p} \text{ [1/s]}$$ (16)

This could be called an extended Arrhenius expression for the ignition time delay of combustible gases. Please relate to equation (1) and (2).

- R is the ideal gas constant
- T is the temperature
- M is the molar mass of the gas mixture
- p is the pressure
- B is a positive constant

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 E by data fitting.

The values for *A*, *E*, *C* and *D* are found at high temperatures and small residence time, thereby neglecting the second term on the right side of the equation. The value of *B* is found at the tabulated autoignition temperature for the gas mixture, i.e. when the ignition time is infinite.

The interpretation of equations (15) and (16) is as follows. The **first term** on the right side is due to chain branching and production of radicals 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 ignition temperatures with very high residence time, τ_{ign} is very large and decay and production of radicals are equal (corresponding to left side = 0). This relates to Figure 1. For high temperatures all graphs of this figure have straight lines (left side of graphs). However, at certain low temperatures all graphs approach asymptotically a separate vertical line with infinite ignition time, which corresponds to solving equation (16) for T with left side = 0.

Experimental setup with hot steel pellet in gas flow

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

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

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

An overview of the test rig with the test object is shown in Figure 3. The height of the test rig is about 2 m and the test object has the height of 16 cm.
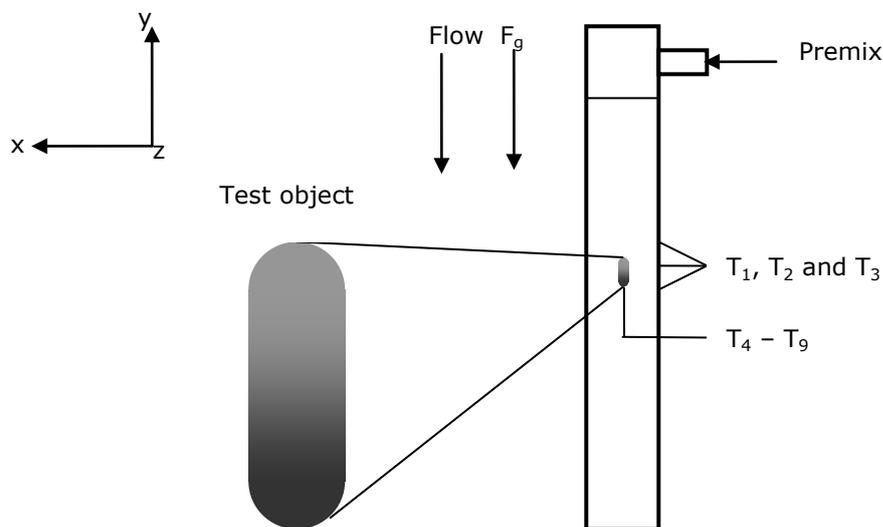

Figure 3   Overview of the geometry of the test rig

The flow of premixed gas/air was from top and down. Figure 4 and 5 show the test pellet installed in the test rig, cold and glowing, respectively.

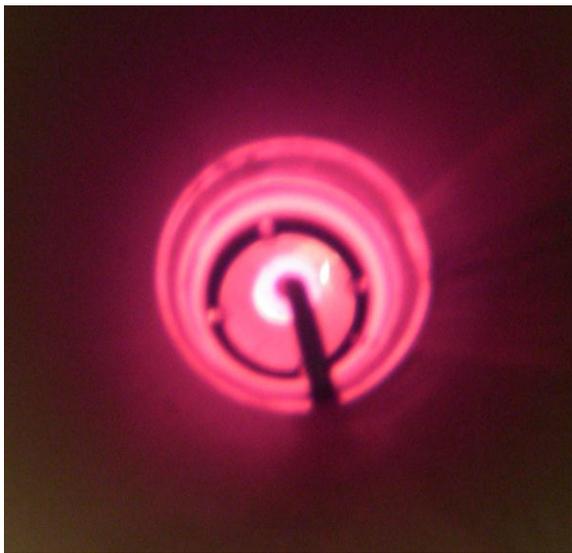*Figure 4   Cold test object in test tube*

Figure 5   Glowing test object in test tube

Results of CFD modelling and experiments

The cases of the test setup were modelled by CFD solving the balance equation (4) with equation (15) giving the source term for I_{gn} at ignition conditions. I_{gn} is solved for in the volume of interest. If at any point I_{gn} exceeds 1.0, ignition will occur.

On the other hand, a hot body in the volume of interest could be adjusted in temperature until the calculations show only one point with I_{gn} above 1.0, which then indicates the maximum temperature (or just below) of the hot body to avoid ignition in that volume of interest.

The residence time τ is solved for like I_{gn} but with density ρ as the source term.

The boundary conditions for both τ and I_{gn} are zero at inlet and "adiabatic" at solid walls.

The CFD modelling includes flow of the premixed gases, heat transfer and thermal radiation. The radiation model used is the CRG model /4/.

Ideally, the results for I_{gn} should end at 1.0 as maximum in the calculation volume in each case. Table 1 shows the actual results for Max I_{gn}.

To estimate how much the CFD model is on the conservative side, the temperatures for the test object were reduced in the modelling cases 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 I_{gn} of 1.0 along the heated test object. Figure 6 shows examples of CFD results in case 2.

Test	Natural gas in air [%vol]	Residence time [s]	Test object mean temp. [K]	First results Max. I_{gn} [-]	With reduced temperatures 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

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

It should be noted that the "Residence time" of Table 1 is the calculated difference of τ from the point where the flow hits the pellet until the ignition point with maximum I_{gn}. τ in Figure 6 is the absolute residence time from inlet of gas flow above the pellet.
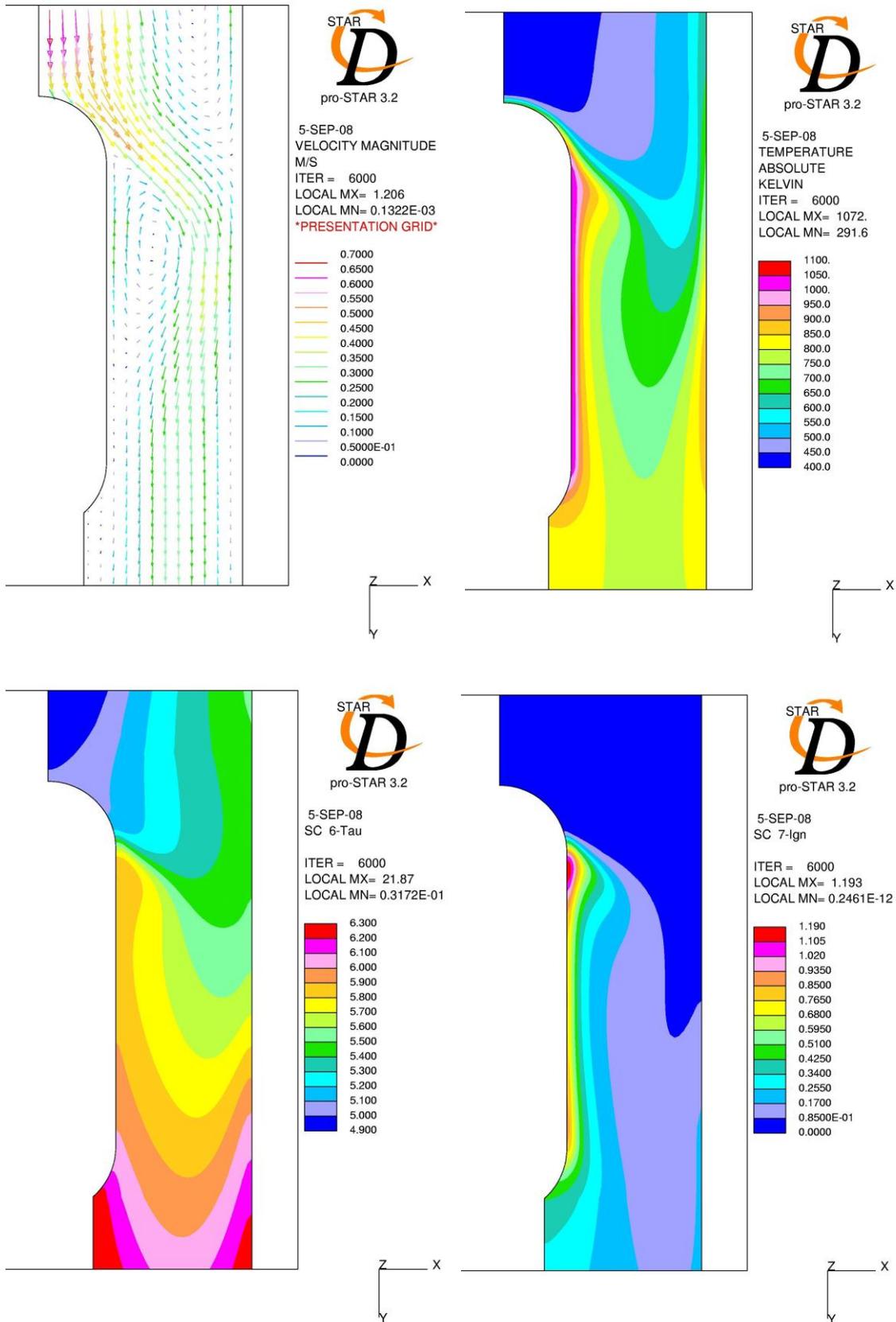
Figure 6   Examples of CFD results

The present work has shown that by using this simple one-equation model a very good representation of the ignition time delay (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 actual test cases within deviations of only 0-50K and on the lower side. These deviations include all the possible uncertainties from the CHEMKIN modelling, from the derived one-equation model, from the experimental data and, finally, from the CFD modelling of the experimental setup.

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.

Conclusions

The model of the Ignition Parameter is a novel model, which gives very good results and may be a great help in predicting probabilities 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 probability of autoignition for natural gas near a heated surface in relation to a given natural gas/air mixture within the explosion limits.

The model of the Ignition Parameter could be used in all cases where it is desired to know the probability of ignition of a gas/air mixture. 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.

Acknowledgment

References

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