SAFe and Efficient hydrocarbon oxidation processes by KINetics and Explosion eXPertise and development of computational process engineering tools

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Introduction

This deliverable reports recent advances in modeling of explosion indices. First phase of the task was building the structure of the program and filling it with core procedures and functions [22]. Now the sub-models are under development. The most important of them are the models for: burning velocity, obstacles, heat transfer. Additionally, procedures calculating transport properties of the mixture are being added. These are necessary for calculating such parameters as Reynolds number. Also a number or minor improvements has been made. They should make the program more user friendly and flexible. An especially large effort was made to develop a convenient, simple and intuitive user interface. Also some data were collected. They are used as a input data and will create a database which will be a part of the software package.

Although the title of this report consists of many topics the report is mainly focused on modeling of turbulent burning velocity. It turned out, as was expected, that burning velocity is the variable of great importance and extremely hard to model. Detailed analysis of literature data has shown that there are significant differences between publications even for laminar burning velocity. The situation gets worse when turbulent burning velocity is analyzed. Therefore more time was spent on studying this crucial problem. Especially the case of spherical flame was investigated. Also some extra experimental work was done to cope with this problem. Measurement of pressure and flame radius as function of the time allows developing a more accurate model of laminar and turbulent burning velocities for methane-air mixture. Also the relation between turbulence and burning velocity was carefully studied. One must stress here that although there is a lot of such data in literature, it is very difficult to create an accurate, general model for a whole set of combustible mixtures. Each gas must be treated separately.

When the model of turbulent burning velocity was set up (for methane) next step was the model of interaction between the flame and obstacles present in the vessel. This part of work is at an initial stage and still demands an extensive literature analysis and more simulations. Probably CFD simulations will be needed to create sub-models of a few most common types of obstacles.

The structure of the code allows simulating of explosion in vessels of different shapes. At the beginning of the project, a model of spherical vessel has been developed. Next it will be expanded to elongated vessels. Various shapes of the vessels results in various shapes of the flames. Although this is basically a geometrical issue, it affects other phenomena like accelerating of the flame or heat losses to the walls of vessel. The report shows which particular sub-models are affected by the change of geometry and how they are going to be extended.

The program has also the possibility of modeling explosion in a branched installation which consists of several vessels. This feature was built in the code, but it is not planned to be extensively studied because of complexity of this problem and limited time of the project. The report describes basic principles of this model and directions of possible developments.

Fuel type and concentration

The type of fuel is the most important factor which decides about the course of a possible explosion. First of all it influences laminar and turbulent burning velocities and decides about dynamics of the explosion. In practical applications many kind of fuel are used. Also substances, which are not intended to be a fuel in a given industrial process, can become the fuel in some untypical, accidental situations when ignition source occurs. Thus the program
which simulates industrial explosion should be able to model burning of any possible fuel. Obviously it is practically impossible because of lack of suitable data for each burnable compound used in industry. Therefore the program was designed as a set of sub-models which are or will be as much general as possible at current state of our knowledge. All parameters which describe specific features and behavior of a given combustible mixture are stored in input data files. This approach allows easy extension and modification of the data in the future, even by the user.

It is assumed that the modeled vessel can be filled with one of the predefined mixtures e.g. methane-air, which properties are defined in mixtures database. The parameters which must be provided with the mixture type are:

- equivalence ratio
- dilution ratio
- initial temperature
- initial pressure

Additionally the files with data about the mixture, thermodynamic data and transport data must be provided. These information are written in the `input.ist` file, listed below (red highlighted). Full description of input files will be given at the end of project when final version of the program is obtained.

Listing 1. The input file defining the problem

```plaintext
Installation****************
Name:                The plant
t_end:               10.00
dt_save:             0.001
Vessel****************
Name:                Bomb1250
kind:                sphere
size:                0.668
pos_ign:             0.0
ignited:             1
Fresh_mixture*******
Mix_Data_File:       Mixtures.mix    
Th_Data_File:        THERMO.DAT      
Tr_Data_File:        TRANSPORT.DAT   
Mixture_name:        H2-air
equiv_ratio:         2.3
dil_mol_frac.:       0.00
init_temp.:          300.0
init_press.:         1.0
Products_mixture*****
Th_Data_File:        THERMO.DAT      
Tr_Data_File:        TRANSPORT.DAT   
Pr_list_File:        product.lst     
Vessel_end**********
here, the comment
can be
Installation_end*****
```

When the type and composition of the mixture is set up, the program looks for the mixture data in the specified file e.g. `Mixtures.mix`. This set of data describes:

- composition of the fuel,
- composition of the oxidizer,
• composition of the diluents,
• set of coefficient used for calculation of the laminar burning velocity,
• set of coefficient used for calculation of the turbulent burning velocity,
• limits of the validity of the above data

In a single file many type of mixtures can be stored. An example of description of a multi-fuel mixture is given here (Listing 2).

Listing 2. Set of data defining the mixture.

Mixture_name: HC-air-CO2
Species_in_fuel: CH4 C2H6
Fuel_composition: 0.9 0.1
Specie_in_oxidiser: O2 N2 Ar
Oxidiser_composition: 0.21 0.78 0.01
Specie_in_diluent: CO2 Ne
Diluent_composition: 0.8 0.2
Z: 1.0
W: 0.422
n: 0.15
zeta: 5.18
alfa_T0: 2.0 300.0
beta_p0: -0.5 100000.0
f: 2.3
turb_f_s_Rec_theta: 4000.0 0.39
fi_limits: 0.0 100.0
F_limits: 0.0 100.0
T_limits: 200.0 500.0
p_limits: 0.1 100.0

When the type of mixture and its properties are taken from the file, the program reads the thermodynamic and transport properties of the species which are present in the mixture. The program uses Chemkin [32] format files for this purpose.

This type of representation of the mixtures is very flexible and, on the other hand, it is able to handle even very complicated behavior of the mixture. Although only two parameters describe turbulent burning velocity in the example (Listing 2, Re, θ), it is possible to use many factors in the file. The final form of the input files will be fixed when all sub-models are finished. Details will be explained later. It is planned to deliver a basic set of mixtures but the user can also define own mixtures. Another advantage of this kind of mixture definition is convenience of handling a few models of the same mixture, according to different references. Obviously it should be avoided in direct industrial application, where the abundance of the mixture models could be confusing.

**Turbulence, obstacles and burning velocity**

Generally, good correlations for laminar and turbulent burning velocities are difficult to obtain. Such data can be taken from experiments or numerical simulations. But the first approach is limited by huge number of potential fuels, initial conditions, equivalence ratios. The second method is more flexible, but its accuracy is limited. These problems cause the development of the model to go in two complementary directions. Firstly authors have made attempts to create the most universal model of the burning process, which would be able to handle big number of fuel types in practical situations. Secondly sets of data for the most important cases will be worked out and validated e.g. data about methane-air mixture.
**Laminar burning velocity**

The laminar burning velocity is basically a mixture property, which lays at the roots of many other features of the burning mixture. Thus it is of great importance to use a proper value of this parameter in simulations. The laminar burning velocity is a function of several parameters. The most important are composition of the mixture, temperature and pressure. The composition is typically represent by equivalence ratio $\Phi$ and dilution ratio $D$. Many equations have been proposed to take this into consideration. In the presented model the laminar burning velocity is calculated by use of the most general equation proposed by Gulder [17]:

$$u_l = u_{\infty} \Phi \left( \frac{T}{T_0} \right)^{n} \left( \frac{p}{p_0} \right)^{\beta} \left( 1 - f D \right),$$

Eq. 1

where

$$u_{\infty} = Z W \Phi^n \exp \left[ - \xi (\Phi - 1.075) \right].$$

Eq. 2

The coefficient $Z, W, n, \xi, \beta, \alpha, f, T_0, p_0$ are defined for a specific mixture.

Unfortunately one can not find one universal set of coefficients for a given mixture for a wide range of conditions. Even for the well known case of methane-air mixture, there is no single result. Proposed coefficients [16, 25, 17] show significant discrepancies. The biggest differences has been found for data provided by Gulder [17] and Liao [25]. As illustrated in Fig. 1, one can see, that the difference in some cases is almost 30%. This shows that although the laminar burning velocity depends only on known physical and chemical properties of the mixture, the variability in values is still large. This fact caused additional experiments to be carried out. The goal was obtaining experimental data for methane-air mixture which were used for selection and validation of one of the mentioned relations for the laminar burning velocity.

![Fig. 1 The relative difference between laminar burning velocities predicted by Liao [25] and Gulder [17] for different equivalence ratio and initial conditions.](image)

The 1.25m³ vessel was used in the experiments. Pressure and flame position were measured. A piezoelectric sensor measured the pressure while special, micro thermocouples were used for measuring the flame position. More detailed description is in [31]. Three
models of laminar burning velocity of methane-air mixture were selected to compare with experimental results. The pressure-time curves were selected as a comparing criterion. The following relations for $u_l$ were tested:

- **First relation**, the laminar burning velocity proposed by Gülder [17]:

\[
    u_l = u_{l0} \left[ \Phi \left( \frac{T}{T_0} \right)^{\alpha} \left( \frac{P}{P_0} \right)^{\beta} (1 - fD) \right],
\]

where

\[
    u_{l0} = ZW\Phi^a \exp \left[ -\xi(\Phi - 1.075)^2 \right].
\]

$Z=1$, $W=0.422$ m/s, $\xi=5.18$, $\eta=0.15$, $f=2.33$ for methane/air mixture.

- **Second relation** proposed by Liou et al. [25]:

\[
    u_l = u_{l0} \left( \frac{T}{T_0} \right)^{\alpha} \left( \frac{P}{P_0} \right)^{\beta} \tag{3}
\]

with

\[
    \begin{aligned}
    u_{l0} &= -34.505\Phi^6 + 212.02\Phi^3 - 528.74\Phi^2 + 682.76\Phi + 481.66\Phi^2 + 177.19\Phi - 26.698 \\
    \alpha &= 5.75\Phi - 12.15\Phi + 7.98 \\
    \beta &= -0.925\Phi + 2.0\Phi - 1.473
    \end{aligned} \tag{4}
\]

- **Third relation**: proposed by Coppens et al. [13] for methane-air mixture with addition of hydrogen:

\[
    u_{l0} = \left( 1 + \gamma \xi^2 \right) W\Phi^a \exp \left[ -\xi(\Phi - 1.06)^2 \right] \tag{5}
\]

where:

$W=0.372$ m/s, $\xi=5.18$, $\eta=0.15$, and $\alpha=0$ in our case there is no hydrogen.

Next three plots show comparison of calculation with experiments for three equivalence ratio. The calculation were done with assumption that the combustion is laminar all the time.
Fig. 2. Comparison of the pressure obtained from the laminar model and the experiments, equivalent ratio equal to 0.72.

Fig. 3. Comparison of the pressure obtained from the laminar model and the experiments, equivalent ratio equal to 1.
Brief analysis of the results showed that first and third relations overestimate the burning velocity and pressure rise ratio for some equivalence ratios. In a more realistic case where turbulent flame has been included they would have failed completely. Therefore the second relation will be used in further calculation for methane-air mixture. It is necessary to rewrite the relation for $u_\nu$ in the form of Eq. 2 to preserve the universal format of input data. It was done by setting parameter $W$ as a polynomial function of $\phi$

$$W = W_0 \sum_{i=0}^{n} a_i \phi^i,$$  \hspace{1cm} Eq. 6

where coefficients $a_i$ are different from those in Eq. 4 and have to be adjusted by any method.

Obviously the problem of most suitable relation for laminar burning velocity is not closed and it still demands more research. Even less clear situation exists for other gases, which have been less studied. The situation can be improved by developing a reliable numerical tool for predicting the laminar burning velocity for various mixtures at different physical conditions. This is one of the tasks of Safekinex project [1].

**Turbulent burning velocity**

Modeling the turbulent burning velocity is probably the most difficult part of the whole model. This is because one has to calculate two phenomena:

- generation of turbulence in flow induced by a moving flame,
- influence of the turbulence on the burning velocity.

The problem was split into two parts because of its complexity. First of all a good model of freely propagating turbulent flame must be obtained. Next it will be extended to the case of interaction with obstacles to the flow and other phenomena which increase the turbulence. According to that the last few months were spent on testing different models for calculating turbulent burning velocity of the flame in the vessel without any obstacles.

The first tested approach is very simple and widely used in many similar models [8, 30, 34 and many others]. The main idea is to connect the turbulent burning velocity $u_t$ with the laminar burning velocity $u_l$ and Reynolds number $Re$. The following relation was used here
\[ u_t = u_l \left( \frac{\text{Re}_c}{\text{Re}_c} \right)^\theta, \]  
Eq. 7

where \( \text{Re}_c \) is critical Reynolds number for given mixture, \( \theta \) is also coefficient characteristic for the mixture. The Reynolds number is defined with respect to laminar flame speed and flame radius \( R_f \)

\[ \text{Re} = \frac{u_l R_f}{\nu_u}, \]  
Eq. 8

\( \nu_u \) is kinematics’ viscosity of the fresh mixture.

Such approach seems not to be consistent with the proposition expressed in the First Report [22, Eq. 30] where the following relation was written

\[ \frac{u_t}{u_l} = f \left( \frac{u'}{u_l} \right) \]  
Eq. 9

or more detailed for methane

\[ \frac{u_t}{u_l} = 1 + a \left( \frac{u'}{u_l} \right)^n. \]  
Eq. 10

But it is very easy to transform Eq. 7 into Eq. 9 or Eq. 10 by using

\[ \frac{u'}{u_l} = f^{-1} \left( \left( \frac{\text{Re}}{\text{Re}_c} \right)^\theta \right) \quad \text{or} \quad \frac{u'}{u_l} = \left\{ \frac{1}{a} \left[ \left( \frac{\text{Re}}{\text{Re}_c} \right)^\theta - 1 \right] \right\}^{1/n}. \]  
Eq. 11

The information about turbulence intensity \( u' \) is necessary in case of obstacles acting on the flame (see next chapter).

Another advantage of this kind of relation (Eq. 7) is its simplicity. It turned out that good correlation of experimental results and calculation could be achieved by setting \( \theta \) as a constant (\( \theta=0.39 \) [9]) and adjusting only one parameter \( \text{Re}_c \). Next graphs show results of this approach. In there are plotted the results of simulation for the turbulent model and the laminar model in order to show influence of the turbulence.

According to Bradley et al. [4] one can assume that for methane-air mixture and for moderate turbulence the Eq. 10 becomes linear with \( a_l=1 \) and \( n=1 \)

\[ \frac{u_t}{u_l} = 1 + \frac{u'}{u_l}, \]  
Eq. 12

then turbulence intensity can be estimated from

\[ \frac{u'}{u_l} = \left( \frac{\text{Re}}{\text{Re}_c} \right)^\theta - 1, \]  
Eq. 13

where \( \theta=0.39 \) and \( \text{Re}_c \) is calculated from an equation derived from experiments

\[ \text{Re}_c = 41323 \frac{s^2}{m^2} \cdot u_l^2 + 1641 \cdot u_l, \]  
Eq. 14

where \( u_l \) is initial laminar burning velocity.
The assumption of moderate turbulence is valid for freely propagating flames if their radius is relatively small. If the explosion happens in large and/or vented vessels where flame radius can rise to several meters and unburnt gas can be accelerated to significant velocity, the assumption can not be valid any longer. Generally it seems that it is impossible to adjust the form of Eq. 9 and Eq. 10 for a whole range of conditions. It is then proposed to use different coefficients for limited ranges of conditions. Drawback is the huge amount of work this can be creates “on demand” for the base of literature data [3, 7] for each specific case.

![Influence of the turbulence in the model. Equivalent ratio = 0.72.](image-url)

Fig. 5. Influence of the turbulence in the model. Equivalent ratio = 0.72.
Influence of the turbulence in the model. Equivalent ratio = 0.83

Fig. 6. Influence of the turbulence in the model. Equivalent ratio = 0.83.

Influence of the turbulence in the model. Equivalent ratio = 1

Fig. 7. Influence of the turbulence in the model. Equivalent ratio = 1.
Influence of the turbulence in the model. Equivalent ratio = 1,3

![Graph showing pressure vs. time for turbulent model, experiment, and laminar model.]

**Fig. 8. Influence of the turbulence in the model. Equivalent ratio = 1,3.**

Influence of the turbulence in the model. Equivalent ratio = 1,42

![Graph showing pressure vs. time for turbulent model, experiment, and laminar model.]

**Fig. 9. Influence of the turbulence in the model. Equivalent ratio = 1,42.**

One can notice that there is relatively good agreement between simulations and experiments for equivalence ratios close to stoichiometric. Also measured and calculated positions of the flame front are in good agreement (Fig. 10). It must be stressed that only the first part of the curves, up to point of inflexion, was compared. At this point heat losses
become important and significantly influence the shape of pressure profiles. A much worse situation occurs for very lean and rich mixtures. At these conditions propagation of the flame is relatively slow and competes with movement of the gas which is generated by buoyancy forces. They deform and move the flame ball upward and the assumption of spherical flame with the center in ignition point is no longer valid. This phenomenon was very well visible when velocity of the flame was compared in horizontal and vertical direction [31].

It is also interesting that the critical Reynolds number is well defined by the initial laminar burning velocity (Fig. 11). If this phenomenon occurs also for other fuel-oxidizer mixtures it will encourage the use of this simple model of turbulent burning velocity.

Although the described method gives good results it is not based on a strong physical basis. Thus another approach, with stronger theoretical background, is also considered. In the previous model the intensity of turbulence is extracted from relation between laminar and turbulent burning velocity and assumed relation between ut and u’. This is a formal operation,
which in fact does use information about a “source” of turbulence. To improve this equation derived by Karlovitz et al. [19] will be used. This equation describes the generation of turbulence by disturbed flame

\[ u' = \frac{1}{\sqrt{3}} \left( \frac{\rho_u}{\rho_b} - 1 \right) u_i \sqrt{1 - \left( \frac{u_i}{u_f} \right)^2} \]  

Eq. 15

The original form of this equation is not able to generate turbulence if the flame is not disturbed or in other words when the flame is laminar. Therefore in this approach the equation is modified by adding a term which triggers the instability and turbulence. The term is related to the critical Reynolds number

\[ u' = \frac{1}{\sqrt{3}} \left( \frac{\rho_u}{\rho_b} - 1 \right) u_i \sqrt{1 - \left( \frac{u_i}{u_f} \right)^2 \left[ 1 - \epsilon \left( \frac{\text{Re}}{\text{Re}_c} \right) \right]} \]  

Eq. 16

where

\[ \epsilon \left( \frac{\text{Re}}{\text{Re}_c} \right) = \begin{cases} 1 \gg \epsilon_0 > 0 & \text{for } \frac{\text{Re}}{\text{Re}_c} > 1 \\ 0 & \text{for } \frac{\text{Re}}{\text{Re}_c} > 1 \end{cases} \]  

Eq. 17

Subsequently the turbulent burning velocity will be estimated from Eq. 9 [7].

This approach is under development and currently results have not been obtained yet.

**Obstacles**

Modeling of an explosion in a vessel with obstacles faces two problems: firstly there is an enormous variety of possible obstacles and its features, secondly there is the requirement of universality of used methods. These two facts force a compromise between generality and accuracy of the simulations. Additionally the models should be well settled on a physical background what will guarantee its flexibility and thus usefulness. The influence of different kind of obstacles on flame propagation has been studied for many years [1, 28, 30, 33 and many others]. It is very complicated problem and many factors are important. Therefore no general approach has been worked out up to now.

Analysis of different methods published in recent years showed that the most suitable approach for this project was used by Arntzen [1]. His subgrid models of generation of turbulence can be easily adopted in our work. The main idea is that every obstacle is a source of turbulent kinetic energy generated by flow inducted by the propagating flame. The turbulent streak interacts with the flame and enhances burning velocity. Second assumption is that obstacles are regularly placed at location which correspond with a given radius of the flame. In other words the interaction is identical on the whole surface of the flame. Also a quasi-steady state of the turbulence is assumed. The turbulent kinetic energy \( k \) is assumed to be a function of drag coefficient \( C_D \) and velocity of the gas \( u_g \) at the moment when the flame approaches the obstacle [1]

\[ k = \frac{a}{2} C_D \sqrt{\frac{A_{obs}}{A_0}} u_g^2, \]  

Eq. 18

where \( A_{obs} \) is the total area occupied by an obstacle at given location (radius), \( A_0 \) is the total cross-section of the channel, or area of the flame. Parameter \( a \) is typically equal to 0.5.
The turbulent kinetic energy describes the strength of the obstacle influence, but it does not provide information about the range of the interaction. The obstacle interacts with the flame as long as the flame propagates in a turbulent streak of the obstacle. Existence of the streak depends on the dissipation rate of turbulent energy $\varepsilon$. The fraction $k/\varepsilon$ represents a time of dissipation $\tau_{dis}$. If $\tau_{dis}$ is known the distance of interaction $l_{obs}$ can be easily calculated from

$$\tau_{dis} = \int_{t}^{t+\tau} u_g dt,$$

where $t$ is the moment the flame passes the obstacle. The dissipation rate can be estimated from the experimental relation [1]

$$\varepsilon = \frac{b}{\sqrt{A_{obs}}} \frac{a}{2} \frac{C_D}{\sqrt{A_0}} \frac{A_{obs}}{u_g^2},$$

where $b=0.3a$.

When $k_i$ is known for all $n$ obstacles, which are in range of $l_{obst}$, and the intensity of turbulence generated by flame itself is $u'_fl$, the overall intensity of turbulence can be calculated from the sum of turbulent kinetic energy

$$u' = \sqrt{\frac{2}{3}} \left[ \frac{3}{2} (u'_{fl})^2 + \sum_{i=1}^{n} k_i \right].$$

The obtained value will next be used in Eq. 9.

Obviously, the presented approach is very simple and one can have many reservations. However a more sophisticated theory would contain more input data which should be taken from experiments. Such complication would rather make the calculations harder than improve their accuracy. The presented model is at a very preliminary stage of work and probably will be modified. It is expected that some parametric study with use of CFD will be necessary. An important advantage of the model is that it uses parameters $k$ and $\varepsilon$, which are provided by the most commonly applied model of turbulence.

**Elongated channels**

Elongated channels are treated as a kind of vessel. The program has potential capability of modeling vessels of different shapes. The most important feature which distinguishes the various vessels is the shape of the flame (Fig. 12). In a spherical vessel the flame is always spherical. In others vessels the flame is initially spherical. When it touches the walls at some points it is locally extinguished. The flame surface becomes a part of the sphere. In some configurations depending on vessel shape and location of ignition point the flame surface can be even split into several parts. But it is still assumed that fresh mixture is homogenous even if it consists of several regions separated by products. This results in the next important assumption that burning velocity is equal in all parts of the vessel. Practically, the modeling of this problem is a geometrical problem of finding the intersections of vessel walls with sphere representing the flame.

Another problem is the modeling of burning velocity. If relation between turbulent burning velocity and turbulence intensity is well established it should work correctly for vessels of almost any shape (excluding vessels with high ratio of area to volume, when excessive heat transfer can even influence the laminar burning velocity). In such case only the model of generation of turbulence by the flame must be replaced, but this situation is unlikely. It is expected that all kinds of vessel will demand their own model of turbulence and turbulent
burning velocity. Development of such models is very costly and one can not expect that they will be sufficiently developed in this limited project.

![Assumed shapes of the flame in different vessels](image)

**Fig. 12. Assumed shapes of the flame in different vessels a) spherical, b) cubic, c) elongated.**

Next problem is simulating the heat transfer in vessels of different shapes. This is a very difficult task because in the elongated vessels the heat losses occur much earlier. This is due to earlier contact between the hot products and walls.

The last but not least problem is a deflagration – detonation transition. Although in spherical or cubic vessels it is less probable, it is very important in long tubes. However this phenomenon is out of scope of the project it must be considered as a limiting factor. For example the program can inform the user that in particular conditions that onset of detonation is possible.

### Explosion in an multi-vessel installation

Thanks to the object-oriented structure of the program [22], an explosion in multi-vessel installations can be handled. The proposed procedure is as follows.

It is assumed that the vessels are connected by junctions which allow the flow of the gas, both the fresh mixture and the products. The introduced mass of gas is instantly mixed with the contents of the vessel and new parameters of fresh mixture and products are calculated with frozen or equilibrium conditions respectively. If the junction lets products into a fresh mixture the ignition takes place. Next the course of explosion is calculated in each vessel separately. This method has an important limitation. Because the model of vessel can handle only single ignition point in each vessel the structure of the installation must not have any loops. It must be a tree type net. Additionally the change of gas composition in each vessel can not be very significant. If the opposite situation occurs the model of mixture combustion
for a given vessel will not be valid any longer, because this model is attributed to the vessel at the beginning of calculation and it is not modified during calculations.

The model of explosion in multi-vessel installations can be applied if three sub-models are developed:

- model of mass and energy exchange through a junction between vessels,
- model of mixing of fresh mixture and combustion products in all four configurations,
- model of explosion with ignition in an arbitrary (junction) location.

**Summary and plans**

The report has shown recent developments in task 3.7 of Safekinex project. The model of explosion is well defined now, however it demands several extensions and improvements. Recent work has allowed choosing the most appropriate model of a laminar burning velocity for methane-air mixture. Also a relatively accurate model of turbulent burning velocity was developed for this mixture. This was achieved by using extensive numerical simulations and experiments carried out especially for this purpose. Although the results are satisfactory, a new approach was also proposed and is currently studied.

Also a graphical user interface is continuously developed to ensure comfortable use of the program. Other minor improvement is a new procedure which calculates transport properties of species. The procedure uses the Chemkin format [32] of a transport file as a format of input.

The report includes also some propositions of sub-models which are planned to be applied in future. These are:

- model of obstacle-flame interaction,
- model of elongated vessels,
- model of explosion in multi-vessel installations.

These must be treated as a first approach, and subsequently going to be improved and even significantly changed.

Besides the mentioned sub-model a model of heat transfer must be developed in the near future. This is a very important but difficult task.

Incorporating several sub-models into one model of explosion causes several coefficients to be fitted simultaneously. One coefficient can be established manually but for multi-dimensional optimization this means tedious work. Therefore it is considered to create a tool which automates this operation. It could be part of the software package and it could be used by advanced users in order to adjust the models to their particular goals.

**References**


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