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Calculation of Detonation Cell Sizes for Hydrogen-Air-Steam Mixtures at ITER Typical Pressures

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Abstract

Results are presented on detonation cell sizes calculations for ITER relevant mixtures and initial conditions, which are required to evaluate DDT potential. An extended version of GP – software (Gas Properties) is described. This software provides both graphic and tabular representation of various properties of mixtures of hydrogen concerning flammability, explosion properties (including detonation cell sizes), thermodynamic parameters, and transport properties. Calculated values of detonation cell sizes are presented for a range of conditions typical for ex-vessel LOCA scenarios in VVPSS. It is shown that generally the detonation cell size decreases with pressure. However, for certain ranges of initial conditions and mixture compositions the function of detonation cell size on the initial pressure is not monotonic. Evaluation of DDT potential, thus, should use detailed analysis of the cell size data. The GP – software gives an efficient tool for such an analysis.

Berechnung von Detonationszellgrößen für Wasserstoff-Luft-Dampf-Mischungen bei ITER-typischen Drücken

Zusammenfassung

Die Ergebnisse einer Berechnung der Detonationszellgröße für ITER-relevante Mischungen und Anfangesbedingungen, die zur Bestimmung des DDT-Potenzials benötigt werden, werden präsentiert. Eine erweiterte Version der GP-Software (Gas Properties) wird beschrieben. Verschiedene Stoffwerte für Wasserstoffmischungen, wie Zündgrenzen, Explosionsstoffdaten (inkl. Detonationszellgrößen), thermodynamische Parameter und Transportstoffwerte, werden sowohl graphisch als auch in Tabellenform ausgegeben. Für Anfangsbedingungen, die typisch für ein VVPSS Ex-Vessel LOCA-Szenario sind, werden Detonationszellgrößen ermittelt. Es zeigt sich, dass die Detonationszellgröße mit steigendem Druck abnimmt. Für einen gewissen Bereich von Anfangsbedingungen und Mischungszusammensetzungen ist der Verlauf der Detonationszellgröße über dem Anfangsdruck nicht monoton. Die Bestimmung des DDT-Potenzials muss daher eine detaillierte Analyse der Zellgrößen umfassen. Mit der GP-Software steht dazu ein effektives Werkzeug zur Verfügung.

Contents

Introduction

Three-dimensional gas distribution calculations for the ITER-VV, the connected SP and the PSS have shown that in ex-vessel LOCA scenarios explosive hydrogen-air mixtures can exist in the in the VVPSS over many hours. Loads that can be expected from various combustion events in flammable hydrogen mixture depend essentially on the combustion regime. Three typical combustion regimes can be distinguished in gaseous mixtures. These include slow subsonic deflagrations, fast supersonic flames, and detonations. Detonations represent the strongest combustion regime, because of the highest overpressures generated by detonation waves (typically of the order of 20 times the initial pressure). It is important therefore to estimate possibility of the onset of detonation or deflagration-to-detonation transition (DDT) under ITER relevant initial conditions.

Various investigators have demonstrated (see, e. g., [6, 7]) that the detonation cell size can be used to describe the critical mixture condition (transition from mixtures for which no DDT is observed to those where DDT is observed) for DDT in gaseous mixtures. The cell size represents a chemical length-scale for the detonation wave. For DDT to be possible, it has been shown that the mixture detonation cell size must be smaller than some characteristic length-scale of the apparatus filled with the mixture. In order to estimate possibility for DDT detonation cell sizes are required for ITER relevant mixtures and initial conditions. The objective of this work is to extend the methods developed for calculation of detonation cell sizes and other important explosion properties of hydrogen mixtures to the range of initial conditions typical for ITER.

This report gives a short description of extended GP – software (Gas Properties). This software provides both graphic and tabular representation of various properties of mixtures of hydrogen concerning flammability, explosion properties, thermodynamic parameters, and transport properties. More precisely possible mixtures include $H_2 - O_2 - H_2O - N_2$ where concentrations, pressure (P) and temperature (T) can vary within the following ranges:

H_2:	0.04	–	0.88,
O_2:	0.03	–	0.21,
H_2O:	0.0	–	0.76,
P (Atm):	0.1	–	7.0,
T (K):	273	–	700.

The range of initial pressures was extended to the 0.1 atm for ITER typical pressures and the 273 K temperature as the low temperature limit was added.

Variables

Full list of properties and variables is given in Table 1. All the properties were pre-calculated and tabulated. The tables were used to generate dynamic libraries COND.DLL, D_H2.DLL, D_O2.DLL, DCJ.DLL, FI.DLL, FL.DLL, LAMBDA1.DLL, PAICC.DLL, PCJ.DLL, SIGMA1.DLL, SIGMAX.DLL, TCJ.DLL, TP.DLL, TV.DLL, VISC.DLL. These libraries provide interpolation of the computed tables and work with program GP.EXE for graphical representations of mixture properties. The dynamic libraries can also be used in other applications, as described in the section 'Advanced operations'.

Calculations of transport properties were made with the TranFit package [2], thermodynamic properties – with CHEMKIN-II package [1], detonation and combustion properties – with STANJAN package, and detonation cell size calculation – with CELL-H2 program [3].

Limits for different explosions regimes were calculated on the basis of approximation for experimental flammability limits [4], flame acceleration criterion [5], and criterion for Deflagration-to-Detonation Transition (DDT) [6].

Limits for flame acceleration (FA) was not extended in the present version of the code to sub-atmospheric initial pressures. Additional experimental data and analysis are necessary to make such an extension possible. The corresponding experimental program is currently underway in according to EFDA Subtask TW2-TSS-SEA 5.4.

Table 1: Variables that are used throughout the program with short descriptions

Main independent variables		
H_2	Hydrogen concentration	
O_2	Oxygen concentration	
H_2O	Steam concentration	
P	Pressure (Atm)	
T	Temperature (K)	
Simple combinations of concentrations		
N_2	$1-H_2-O_2-H_2O$	Nitrogen concentration
$H_{2\ dry}$	$H_2/(1-H_2O)$	Dry concentration of hydrogen
f	$H_2/2O_2$	Equivalence ratio
F	$f/(1-f)$	Normalized equivalence ratio
r	O_2/N_2	Oxygen to nitrogen ratio
R	N_2/O_2	Nitrogen to oxygen ratio
W_{rel}	H_2O/W_{max}	Relative humidity
Detonation properties		
λ	Detonation cell size (m)	
T_{cj}	CJ temperature (K)	
P_{cj}	CJ pressure (Atm)	
D_{cj}	CJ detonation wave speed (cm/s)	
Thermodynamic properties		
σ	Expansion ratio	
P_{aicc}	Pressure after adiabatic combustion in constant volume (Atm)	
T_v	Temperature after combustion in constant volume (K)	
T_p	Temperature after combustion at constant pressure (K)	
W_{max}	Maximum (saturated) H_2O concentration at given P, T	
Transport properties		
Cond	Temperature diffusivity (cm^2/s)	
Visc	Viscose diffusivity (cm^2/s)	
D_{H2}	Diffusion coefficient for H_2 (cm^2/s) in mixture	
D_{O2}	Diffusion coefficient for O_2 (cm^2/s) in mixture	
Explosion limits properties		
FL	Flammability limit — positive values indicate possibility of flame.	
Fast	$\sigma-\sigma_{max}$; Positive values indicate possibility of fast flames.	
DDT	$\ln(L/5\lambda)$; Where L – characteristic size. Positive values indicate possibility of DDT.	
FI	Flame index: 0 – no flame; 1 – slow flame; 2 – fast flame; 3 – fast flame and DDT. Intermediate values (1–2 and 2–3) demonstrate current uncertainty in determination of combustion regime.	
σ_{max}	Criterion for fast flames (fast flame is possible if $\sigma>\sigma_{max}$)	

Coordinate space selection

Program can plot contours of constant values of any variable from Table 1 on 2D subspace of coordinate space: $H_2 - O_2 - H_2O - P - T$. However, it is possible to use combinations of concentrations (except relative humidity) as main variables to some extent. In order to select 2D subspace two main variables should be selected that become X and Y-axis of 2D subspace, and other three variables should be fixed at some constant values. So, total of 5 variables should be selected from list: H_2, O_2, H_2O, P, T, N_2, $H_{2\,dry}$, f, F, r, F. Of course, this choice is not absolutely free. It should be possible to reconstruct main variables given the values of selected variables. There are some restrictions on selection:

      P and T should always be selected.

      Following combinations should not be selected simultaneously:

            F and f;

            R and r;

            O_2, N_2 and R or r;

            H_2, O_2 and F or f;

            H_2, H_2O and $H_{2\,dry}$.

At program start you will get the following coordinate space:

      $X - H_2O$; 0.0–0.8

      $Y - H_2$; 0.0–0.8

      r=const=0.266;

      T=const=300K;

      P=const=1Atm.

User interface

Main window

The Main window shows levels of selected variables in the selected coordinate space. A red cross somewhere in the window shows a "current point". Position of the current point affects information in auxiliary windows. You can set position of current point by mouse click or via menu.

Auxiliary windows

There can be three auxiliary windows in the program: Info, X section, Y section.

The Info window shows values of variables at a current point.

X (and Y) section shows 1D-graphs of selected variables on lines where Y=const (X=const).

Main Menu

The main menu contains the following items:

Submenu 'File' has following items:

'Open' — Opens a file with settings for picture.

'Save' — Saves current settings to a file.

'Save as' — Saves current settings to a file, ask for filename first.

'Exit' — closes program.

Submenu 'Edit' has following items:

'Copy' — Copy content of a window to system clipboard as enhanced metafile.

'Copy to file' — Saves content of a window to enhanced metafile.

Submenu 'View' controls visibility of additional elements: Toolbar, Status bar, Info window, X and Y sections.

Submenu 'Find' has items 'Minimum' and 'Maximum' — moves current point to minimum or maximum of a specified variable

Submenu 'Settings' has following items:

Font — selects font for axis and labels.

Axis — selects 2D subspace for graph.

'Add variable' and 'Variables' — this menu items gives possibilities to select the list of displayed variables; to select range of displayed levels; to choose colors and line styles.

'Sigma max settings' — here you can change coefficients for calculation of σ_{max} — fast flames criterion.

'Lambda level' — here you can enter value of characteristic size that is used in DDT criterion.

'Current point' — here you can change the position of "current point".

Submenu 'Help' contains information about program.

Info window

The Info window contains a list of values of selected variables at the current point. This list should not be exactly the same as the list of plotted variables. However when new variable is added to plot, it is also added to that list. At program start this list contains main variables and λ and σ.

Right to the list are the following buttons:

'Add' — adds variable to the end of list;

'Remove' — removes selected variable from list;

'Move up' and 'Move down' — controls order of variables in list;

'Copy' and 'Copy all' — copies selected or all values to clipboard (in text form).

'Close' — closes this window.

X and Y Section windows

The Section window contains 1D graphs of selected variables on the line Y=const (X=const) though the current point in main window. A Red dotted vertical line shows the position of the current point. A mouse click in the window also moves the current point in the main window. If variables with different dimensions (like concentration:0–1 and temperature:300–700K) are plotted on the same graph (with combined range of 0–700) you will not have a very beautiful graph. To avoid such situations you can change the list of plotted variables. This list can be changed independently from the main window.

The Section windows have the following menu:

'File'
    'Close' — closes window.
'Edit'
    'Copy' — copies content of a window to system clipboard as enhanced metafile.
    'Copy to file' — Saves content of a window to enhanced metafile.
    'Copy as text' — copies data for graphs to system clipboard as text table.
'Find'
    'Minimum' and 'Maximum' — moves current point to minimum or maximum of specified variable
'Settings'
    'Refresh variables' — synchronizes list of plotted variables with main window.
    'Variables' — allows editing list of variables.

Advanced operations

This software consists of the main program GP.EXE and set of dynamic libraries: COND.DLL, D_H2.DLL, D_O2.DLL, DCJ.DLL, FI.DLL, FL.DLL, LAMBDA1.DLL, PAICC.DLL, PCJ.DLL, SIGMA1.DLL, SIGMAX.DLL, TCJ.DLL, TP.DLL, TV.DLL, VISC.DLL. These DLLs should be either in the same directory as GP.EXE or in any directory listed in PATH environment variable.

Each of these libraries represents one variable, as it is obvious from the name of file. These libraries can be used in any software that allows usage of external dynamic libraries.

Each of DLLs has the following entry points:

Entry point	C prototype	Description
_VAR@40	double __stdcall VAR(double H2,double O2, double H2O, double P, double T)	Here 'VAR' stands for real name of variable in upper case. This is the main entry point.
_VMIN@0	double __stdcall VMIN()	Minimum value of a variable
_VMAX@0	double __stdcall VMAX()	Maximum value of a variable
_VNAN@0	double __stdcall VNAN()	Value used to represent absence of data or wrong parameters

Some of libraries have additional entry points:

LAMBDA1.DLL has _LOG_LAMBDA@40 entry point that gives $\ln(\lambda)$. Moreover VMIN, VMAX and VNAN entry points correspond to $\ln(\lambda)$, not for λ itself.

SIGMAX.DLL has entry point _SigMax_@20 with following prototype:

        double __stdcall SIGMAX_(double f, double T, int err)

If err=0 than that function gives the same value as main function (_SigMax@40). When err=±1 this function gives uncertainty range for main function.

FL.DLL has entry points that give the lower and upper flammability limit for hydrogen.

        _LFL@16   double __stdcall LFL(double T, double P)

        _UFL@24   double __stdcall UFL(double T, double P, double r)

An example of software that can use these DLLs is Microsoft Excel. For example: in order to use **Lambda** as worksheet function you should create module in your workbook and add following line to it:

        Public Declare Function Lambda Lib "lambda1.dll" Alias "_LAMBDA@40"
                (ByVal H2 As Double, ByVal O2 As Double, ByVal H2O As Double,
                ByVal P As Double, ByVal T As Double) As Double

Declarations of functions for Visual Basic are in file DLLS.BAS. Declarations for C/C++ are in file DLLS.H. Example for Microsoft Excel are in files DLLS.XLA and DLLS.XLS.

Results of cell size calculations (graphic output)

Results of calculations of detonation cell sizes are presented in Figs. 1 - 13 as examples of GP – software output.
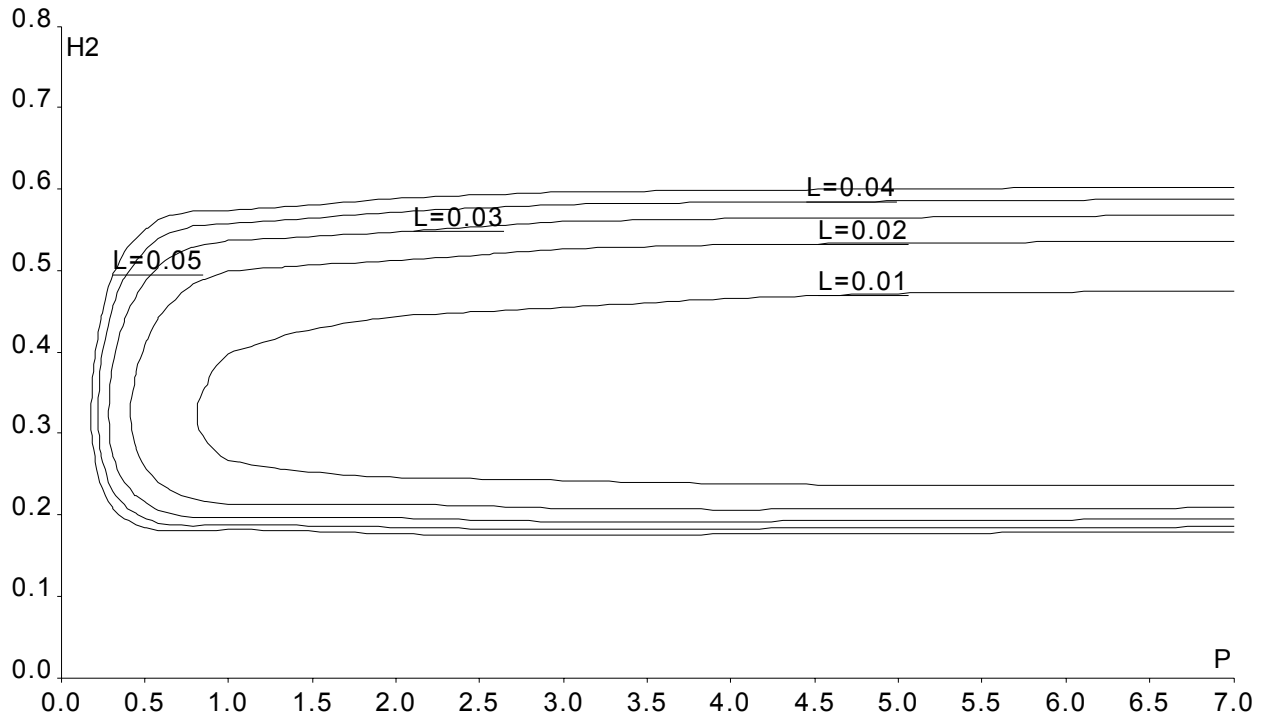

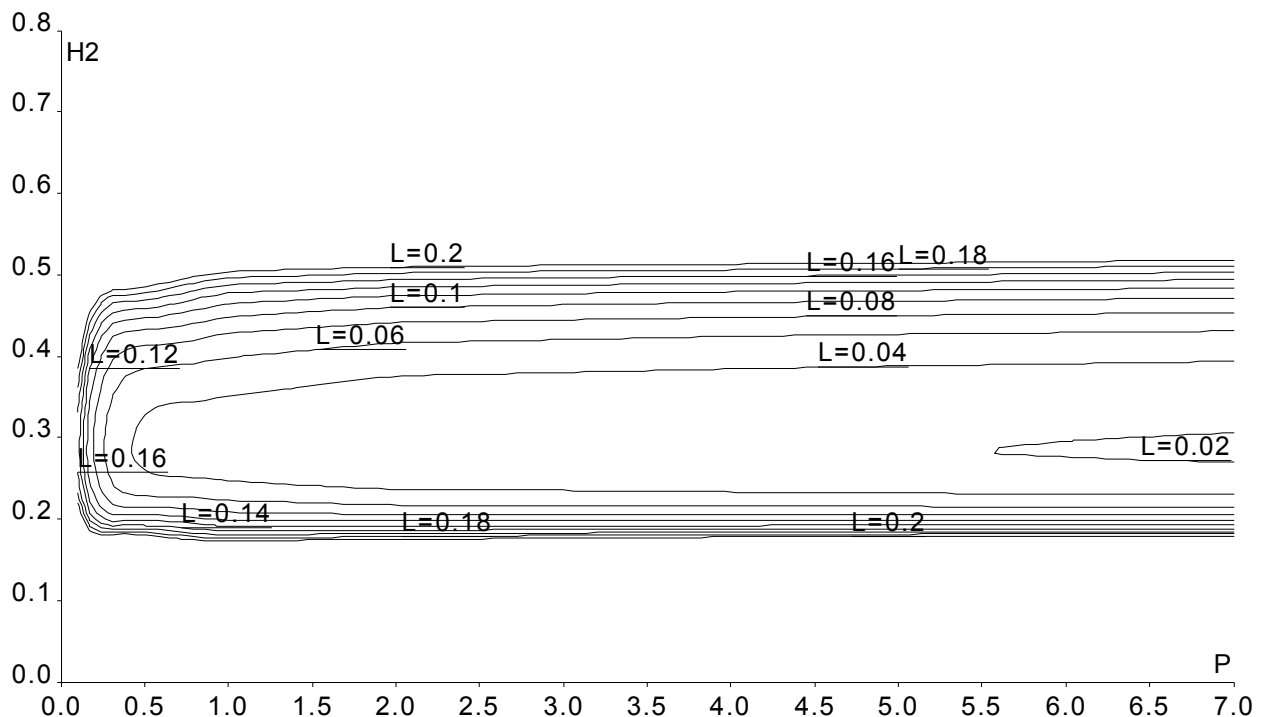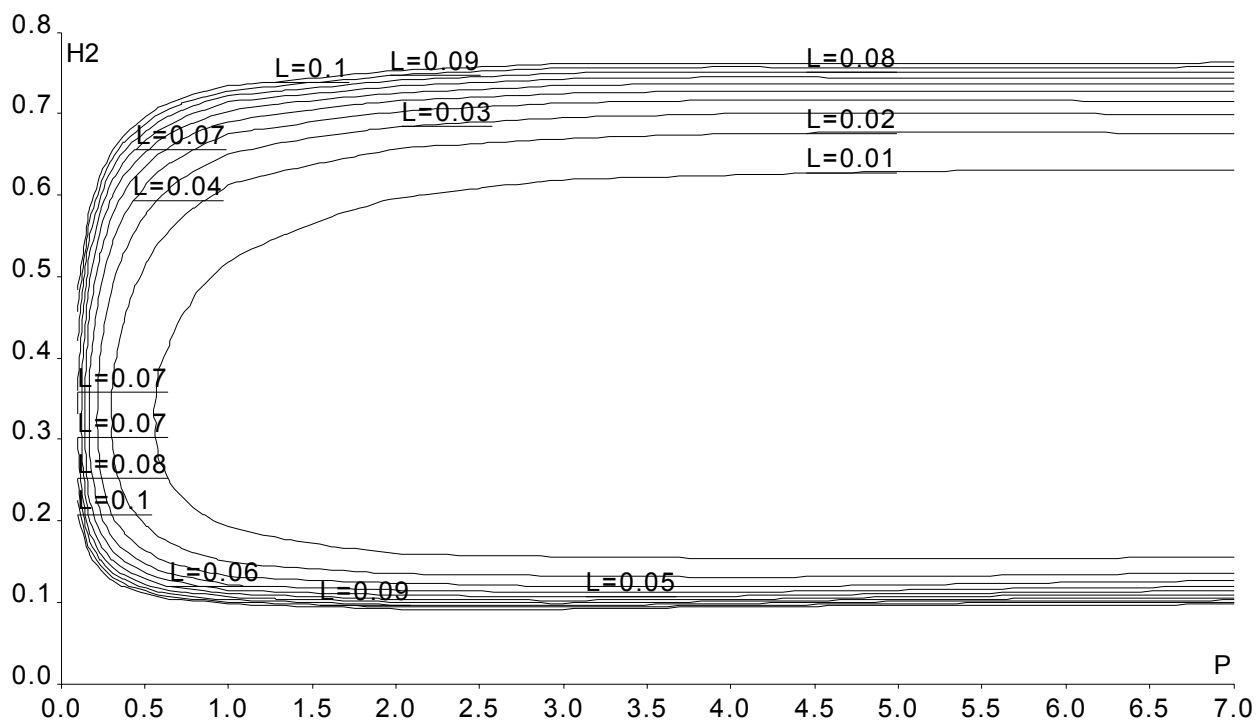Figure 1. Levels of λ (detonation cell size) on H_2-P plane at 373 K, hydrogen-air mixtures.

Figure 2. Levels of λ (detonation cell size) on H_2-P plane at 373 K, hydrogen-air-10% H_2O mixtures.

Figure 3. Levels of λ (detonation cell size) on H_2-P plane at 650 K, hydrogen-air mixtures.
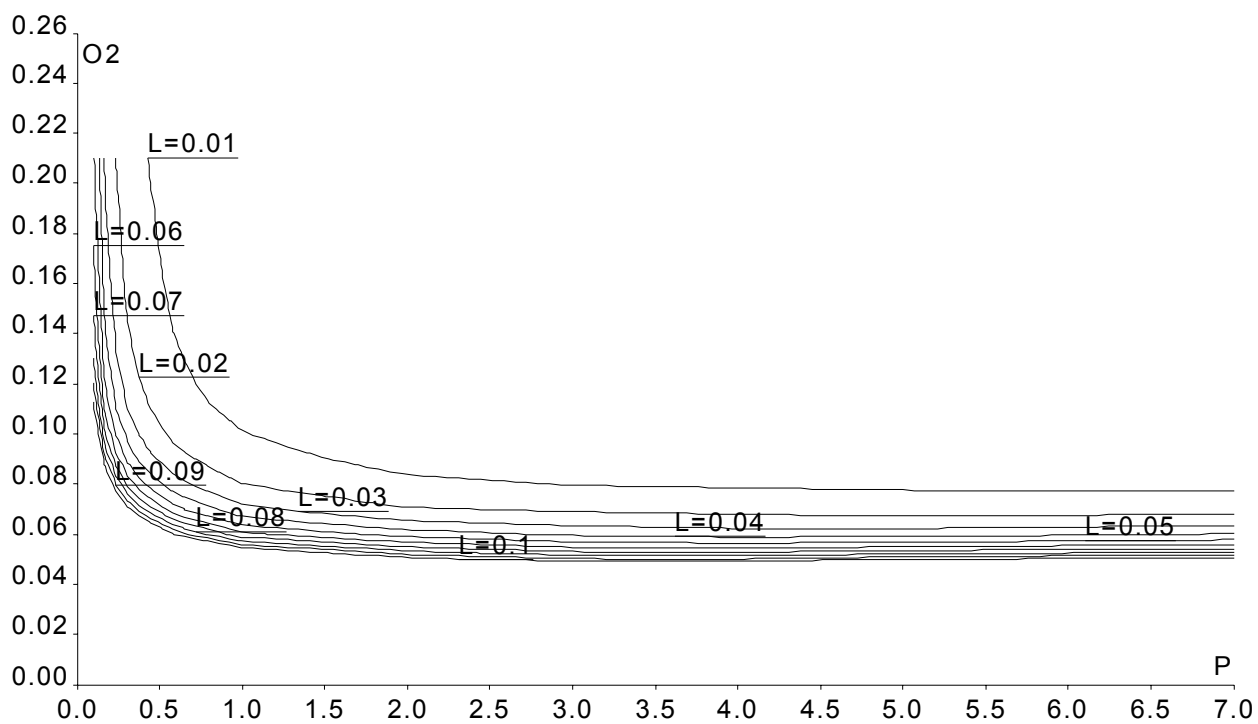
Figure 4. Levels of λ (detonation cell size) on O_2-P plane at 650 K, 30 % $H_2 - O_2 - N_2$ mixtures.
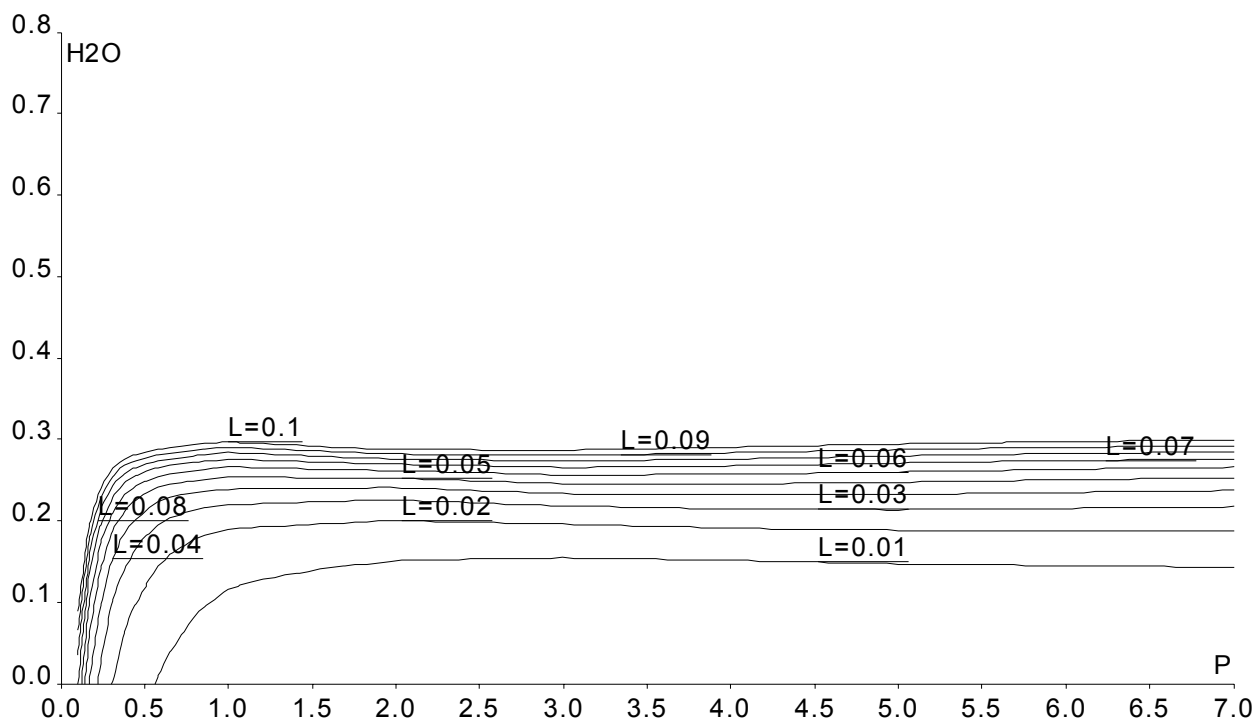
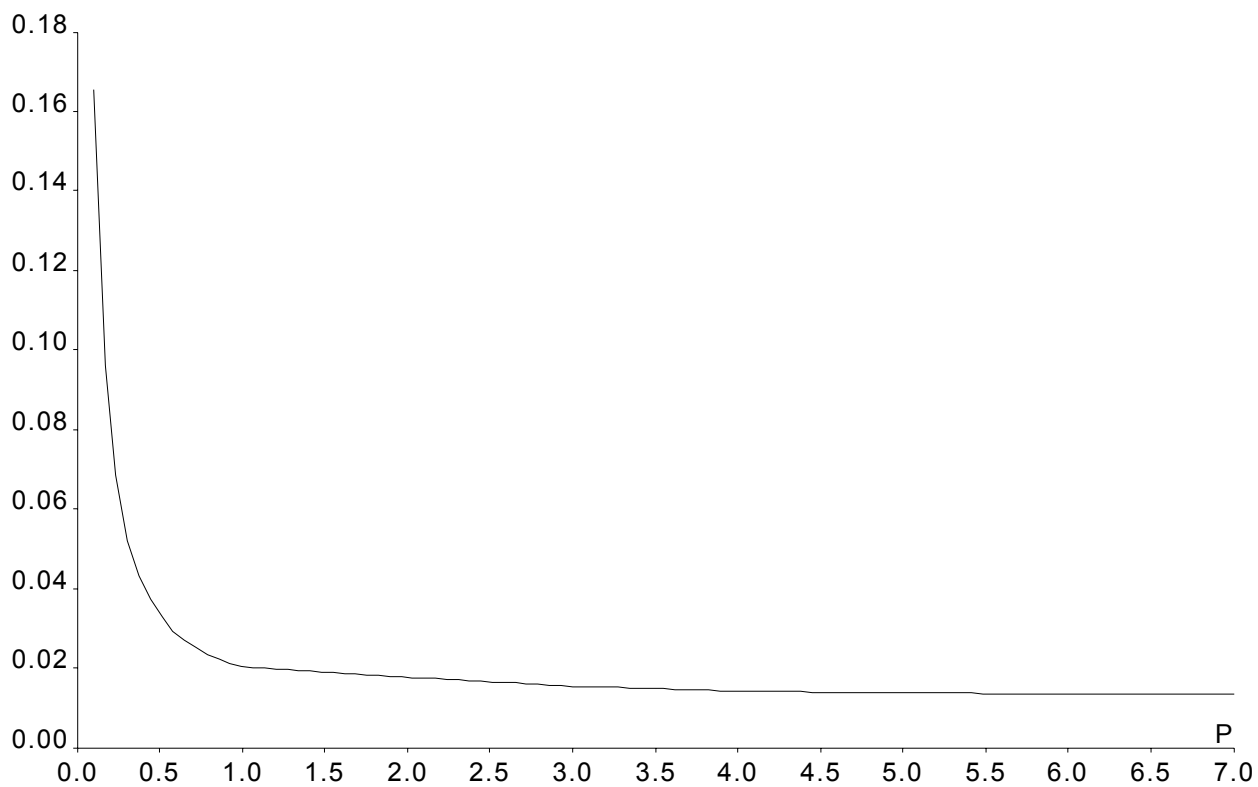Figure 5. Levels of λ (detonation cell size) on H_2O-P plane at 650 K, 30 % H_2(dry) – air – H_2O mixtures.

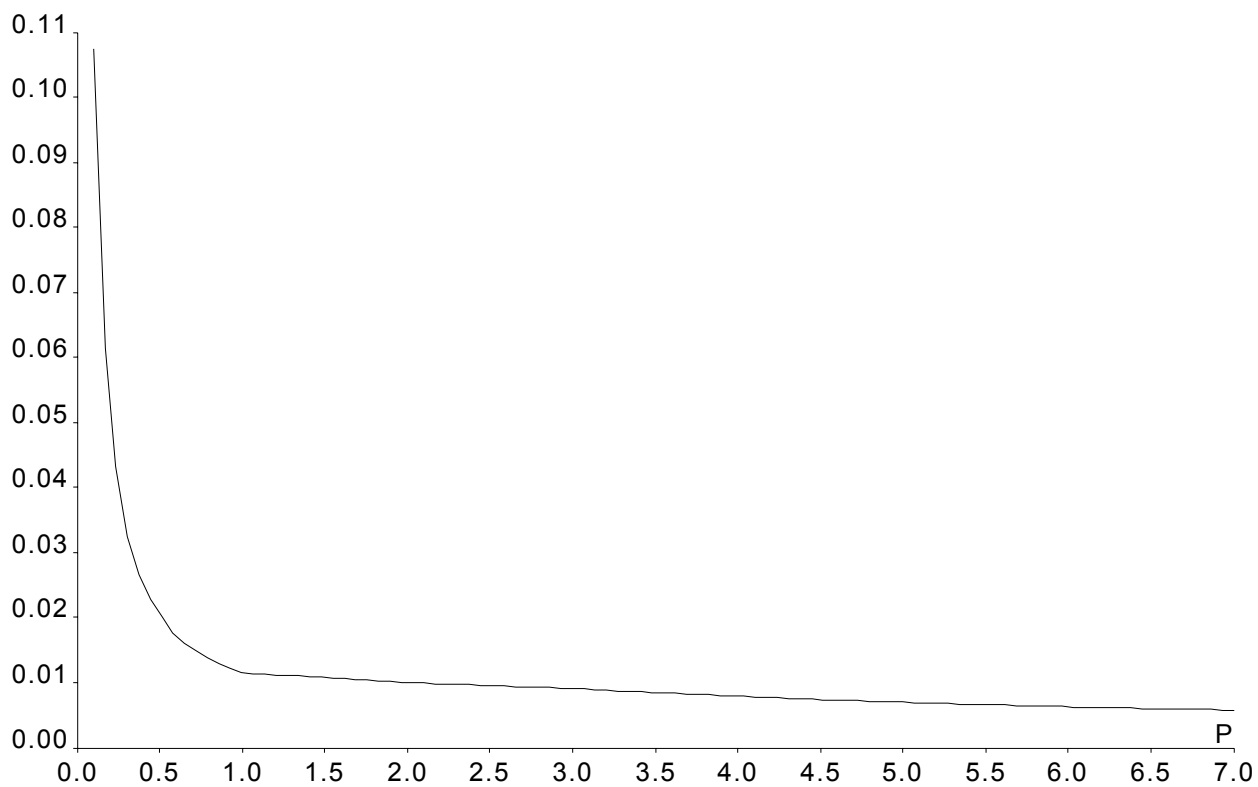Figure 6. Detonation cell size, λ as function of pressure at 373 K, 50 % H_2 – air mixture.

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Figure 7. Detonation cell size, λ as function of pressure at 273 K, 40 % H_2 – air mixture.
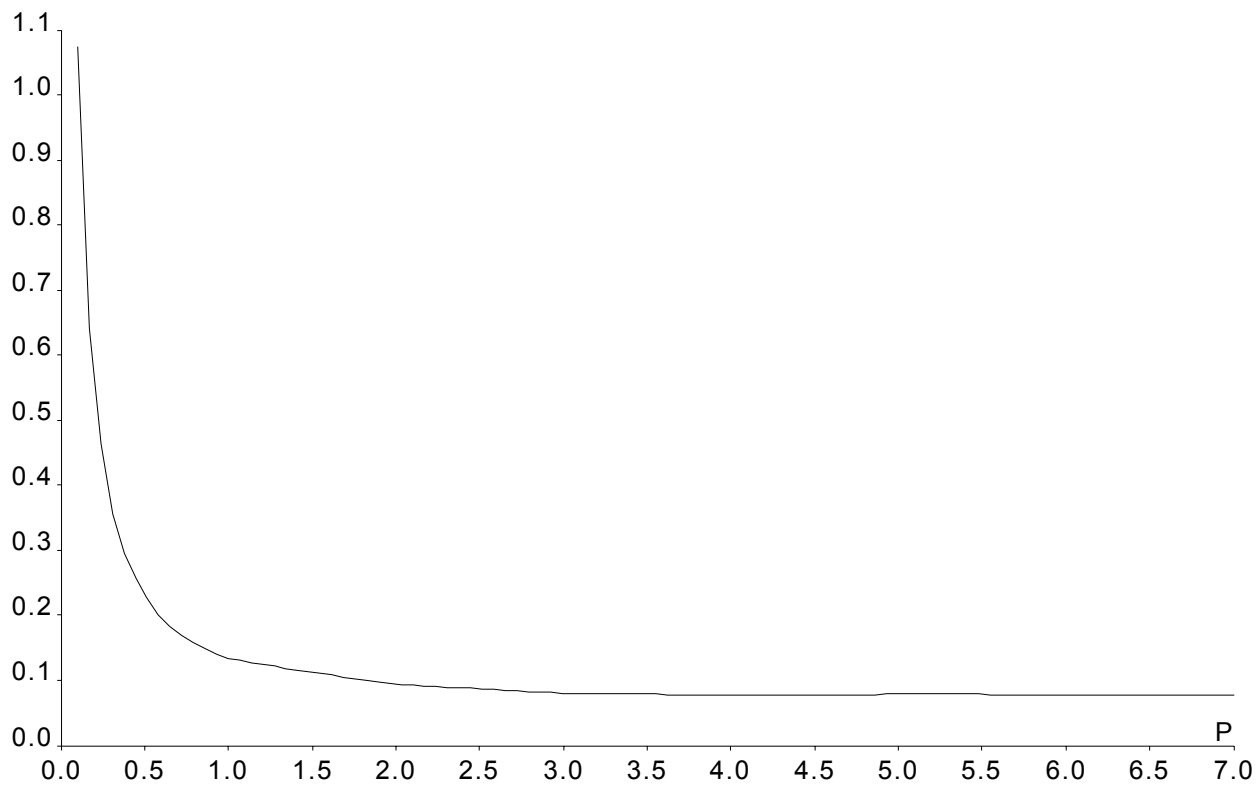

Figure 8. Detonation cell size, λ as function of pressure at 650 K, 75 % H_2 – air mixture.
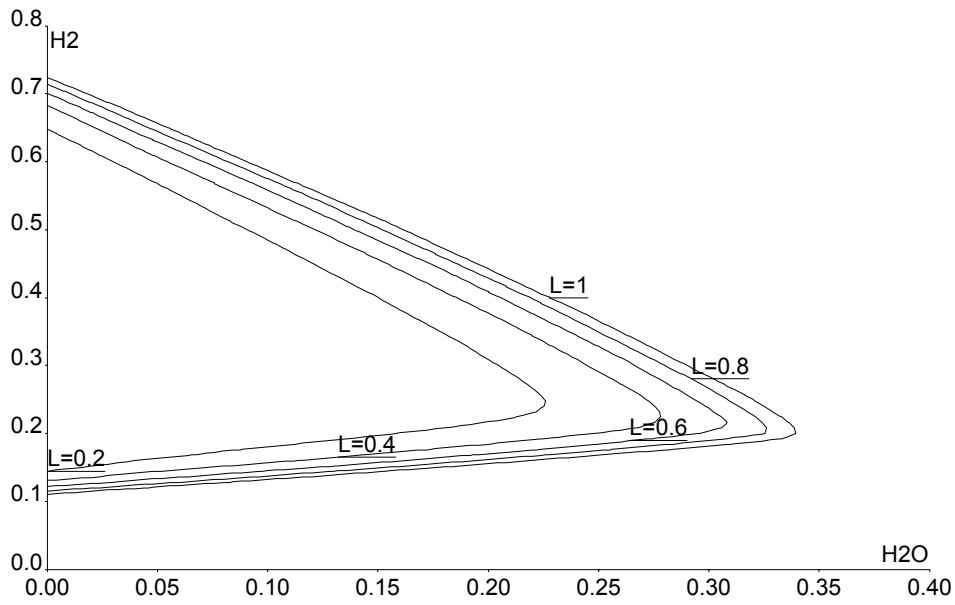
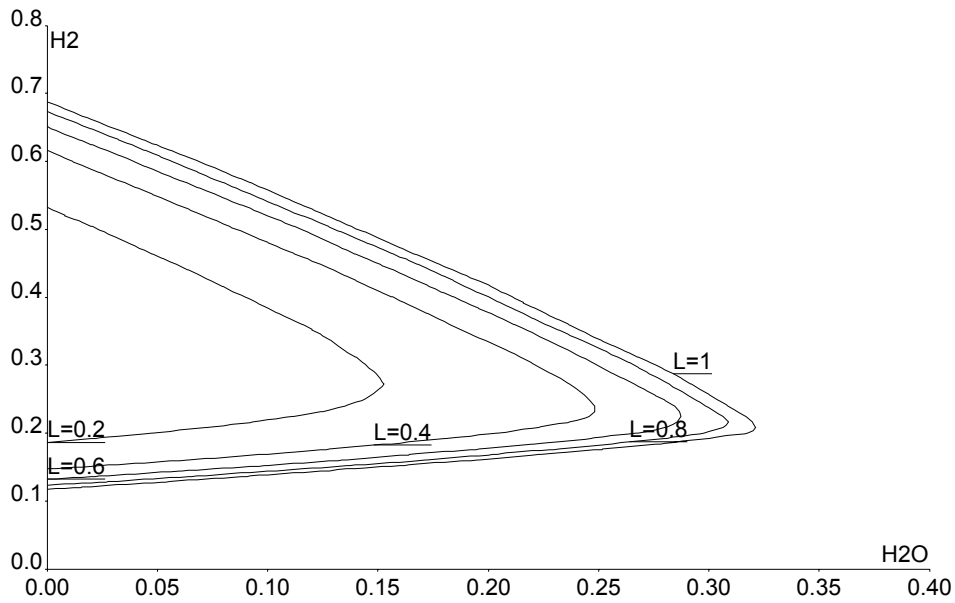Figure 9. Levels of λ (detonation cell size, m) on H_2-H_2O plane at 373 K, p=0.5 bar

Figure 10. Levels of λ (detonation cell size, m) on H_2-H_2O plane at 373 K, p=0.1 bar
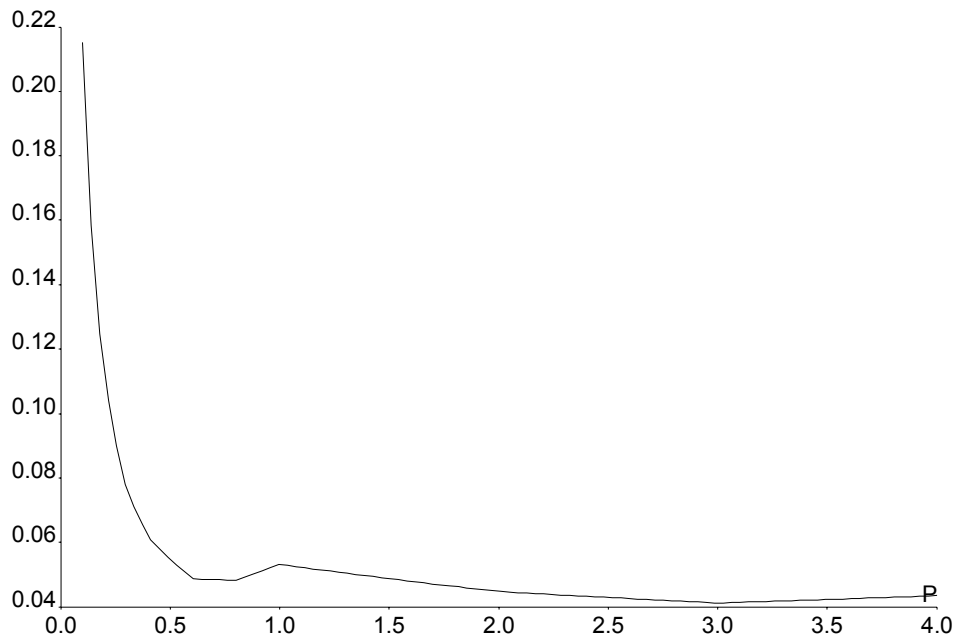
Figure 11. Detonation cell size, λ [m] as function of pressure [bar] at 373 K, 18 % H_2 − 82 % air mixture
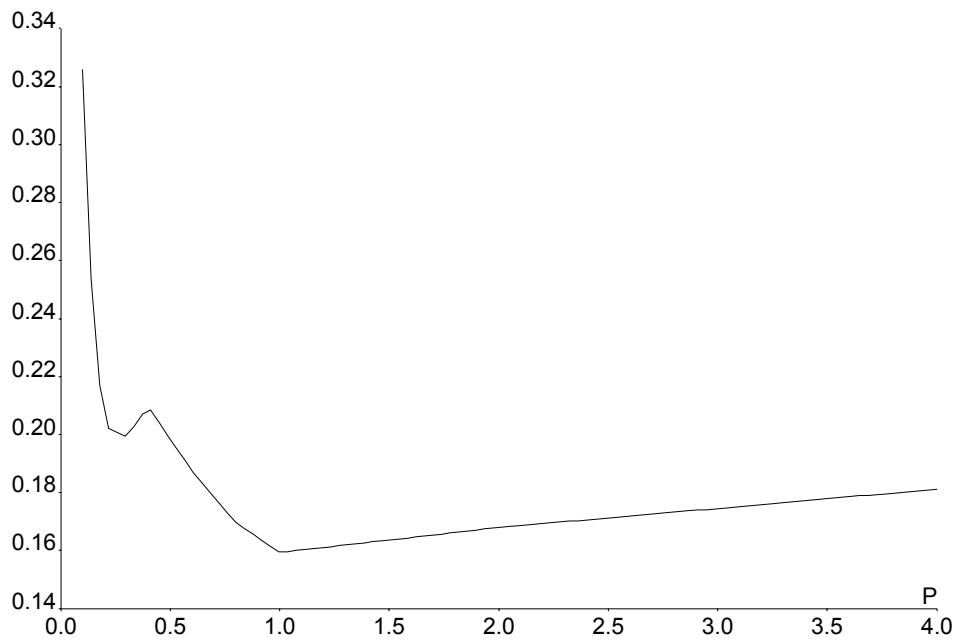

Fig. 12. Detonation cell size, λ [m] as function of pressure [bar] at 373 K, 18 % H_2 − 10 % H_2O − 72 % air mixture
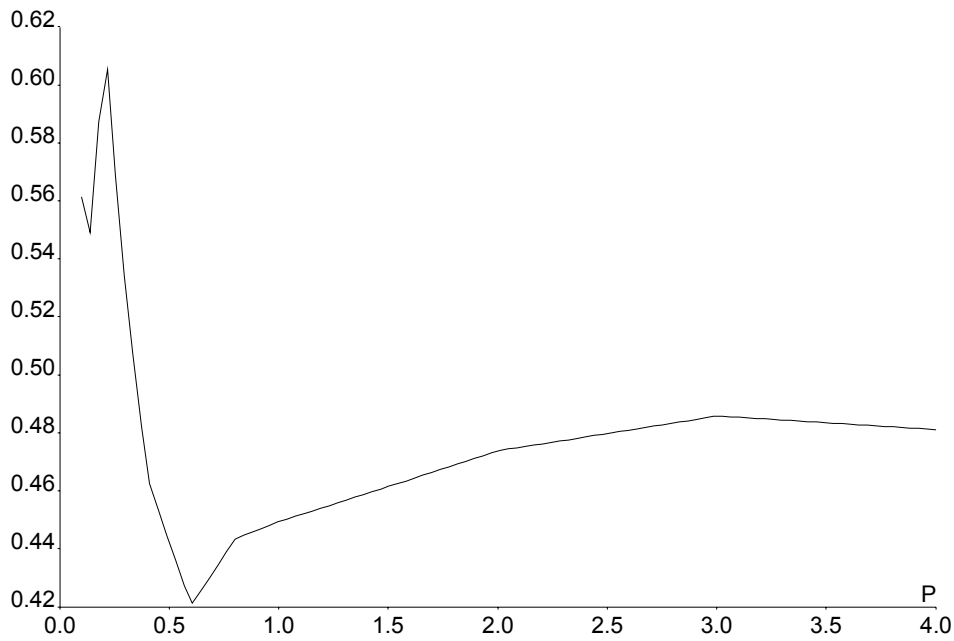
Fig. 13. Detonation cell size, λ [m] as function of pressure [bar] at 373 K, 18 % H_2 – 20 % H_2O – 62 % air mixture

Discussion

Generally, the detonation cell size increases with pressure decrease. This is evident from Figs. 1 – 8. Such a behavior was expected from experimental data known from literature. This means that detonation sensitivity decreases with pressure decrease. Potential for DDT is generally reduced with pressure decrease.

Despite of this general trend for decrease of the detonation cell sizes with pressure, for some mixture compositions the function of cell size on pressure is not monotonic. This is typical for lean mixtures of hydrogen in air (see Figs. 11-13). For certain mixture compositions, pressure decrease below 1 bar results initially in a decrease of the detonation cell size and increase of detonation sensitivity (see Figs. 11 and 13). Further decrease of pressure can lead to the cell size increase and decrease of detonation sensitivity.

These examples show that simple rules, like that detonation cell sizes are inversely proportional to initial pressure, appeared to be not valid for certain range of compositions and initial conditions representative for ITER. Thus estimates of DDT potential should use detailed analysis of the cell size data. The GP software gives an efficient and convenient tool for such an analysis.

Summary

We have presented results of detonation cell sizes calculations for ITER relevant mixtures and initial conditions, which are required to evaluate DDT potential. The work has been focused on extension of the methods developed for calculation of detonation cell sizes and other important explosion properties of hydrogen mixtures to the range of initial conditions typical for ITER.

An extended version of GP – software (Gas Properties) has been developed. This software can get graphic and tabular representation of various properties of mixtures of hydrogen concerning flammability, explosion properties (including detonation cell sizes), thermodynamic parameters, and transport properties. A short description of the software is presented in this report.

Detonation cell sizes have been calculated for a range of conditions typical for ex-vessel LOCA scenarios in VVPSS. It was shown that generally the detonation cell size decreases with pressure. However for certain range of initial conditions and mixture compositions the function of detonation cell size on initial pressure is not monotonic. Evaluation of DDT potential, thus, should use detailed analysis of the cell size data. The GP software gives an efficient tool for such an analysis.

Acknowledgement

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