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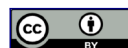
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# Considering Reactions in Design and Simulation of Ejectors

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## Abstract

The influence of gas phase reactions in ejector pumps using gaseous fuel as primary gas is investigated. Simulated ignition delay times are compared to predicted mean residence times of a 1D ejector design tool to investigate if ignition takes place in the ejector tube. 1D results are compared to CFD simulations to take into account non-ideal mixing effects along the ejector.

## Introduction

### Ejector

Ejectors are devices where a high-pressure fluid (primary stream) transfers energy to a low-pressure fluid (secondary stream), entraining the low-pressure fluid and mixing the two streams in the mixing section. When operating the ejector with incompressible fluid (liquids) they are normally referred as jet pumps. When using compressible fluid (gases), the term ejector is generally used (Sun & Eames (1995)).

The design and performance of such devices was subject of numerous investigations over the last years e.g. (Keenan, Neumann, & Lustwerk (1950), Sun & Eames (1995), Lawn (2003)).

When using gaseous fuels (e.g. pure methane or natural gas) as primary stream and air at elevated temperatures as secondary stream, depending on the exact design and conditions, reaction might take place in the mixing section of the ejector. This might lead to off-design conditions for ejectors which are designed to be operated solely under non-reactive conditions.

### Definition of Ignition

To be able to verify if combustion takes place in the ejector, the definition of ignition is very important and is discussed in the following section.

To ignite a mixture a certain amount of energy, in form of heat, has to be introduced to a mixture of combustible material (either gas, liquid or solid) and air (providing oxygen). Different highly reactive radicals are formed, which further react and can then lead to complete combustion of the combustible material.

When talking about ignition, we can distinguish two different ignition initialization processes:

- induced or external ignition (e. g. spark ignition in a petrol engine)
- self-ignition (e. g. diesel engine, gas turbine)

If an flammable, homogeneous mixture of fuel and air, is locally exposed to a, not necessarily constant, high enough temperature (T) and pressure (p), then ignition will take place within a certain time. Fuel (here only gaseous fuel, mainly natural gas, is considered) will react within a very short time (in order of milliseconds) with oxygen contained in the air. This will lead to a sudden temperature increase and, depending on the case, pressure increase. If the released heat of reaction is high enough, then the reaction will continue further without the external addition of energy, till either oxygen or fuel is completely consumed. This process is called self-ignition (Joos (2006)).

### Ignition Delay Time

As ignition is always a transient process, even if the ignition conditions are met, combustion will only take place after a certain ignition delay time  $\tau_{igni}$ . Depending on the exact conditions, the ignition delay time is in orders of micro seconds to up to seconds at the minimum autoignition temperature (MAIT). For methane the ignition delay time at the MAIT (898 K) and at an equivalence ratio  $\Phi$  of 0.5, is in the order of 20 seconds (Reid, Robinson, & Smith (1985)).

### Ignition Delay Time: Experimental

For measuring the self-ignition and ignition delay times of gaseous fuels, often a shock wave tube is used. It consists of a pipe with two chambers, separated by a membrane. One chamber is filled with the fuel/air mixture, the other one with inert gas. Pressure is increased in the inert gas chamber, till the membrane bursts. A shock wave runs through the system and is reflected at the end of the pipe. The shock increases pressure and temperature, which leads to ignition. The ignition delay time is then defined as time from reflection of the shock wave to start of radical formation, more precisely the intersection of the tangent of radical curve and the initial radical concentration. Often CH (431 nm) or OH (308 nm) radical concentrations are measured via chemiluminescence.

Reid, Robinson, & Smith (1985) measured ignition delay time and MAIT of methane/air mixtures using stirred cylindrical (0.5 l volume) and unstirred spherical vessels (0.8 l volume). Temperature inside the vessel was monitored using two thermocouples to define the ignition delay time. The premixed gas has entered the vessel at room temperature and reached vessel temperature in about three seconds. A sharp distinction of ignition and non-ignition was found; a change of 1-2 K of the initial vessel temperature was sufficient to move from ignition to non-ignition.

According to Petersen, Röhrig, et al. (1996) the ignition delay of methane in air can be calculated according to equation (1), for temperatures of 1400 K – 2050 K, an equivalence ratio  $\Phi$  of 0.5 – 2.0 and concentrations of  $[CH_4] < 3.6 \times 10^{-5} \text{ mol/cm}^3$ .

$$\tau_{CH_4} = 4.05 \times 10^{-15} [CH_4]^{0.33} [O_2]^{-1.05} \exp\left(\frac{E}{RT}\right) \quad (1)$$

where  $\tau_{CH_4} \sim p^{-0.72}$ . Here  $\tau_{CH_4}$  is the ignition delay time for Methane in s, E is the activation energy in J/mol (E = 216.8 kJ/mol), R is the universal gas constant and  $[CH_4]$  and  $[O_2]$  are concentrations in mol/cm<sup>3</sup>.

For more accurate predictions Petersen, et al. (2007) suggest different activation energies E according to Table 1. Ignition delay time decreases for increasing equivalence ratio  $\Phi$  (Joos (2006)).

**Table 1** Suggested activation energies E for methane (Petersen, et al. (2007))

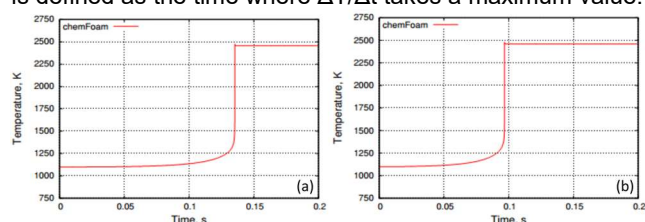
T, K	p <sub>av</sub> , bar	E, kJ/mol
1451 - 2001	0.71	173.7
1407 - 1625	10.9	185.9
1290 - 1407	10.9	151.1
1367 - 1659	19.6	167.8
1243 - 1367	19.6	109.7

Experimental ignition delay times and derived equations for the ignition delay times of C<sub>2</sub>H<sub>2</sub>/O<sub>2</sub>/Ar, C<sub>2</sub>H<sub>4</sub>/O<sub>2</sub>/Ar and C<sub>2</sub>H<sub>6</sub>/O<sub>2</sub>/Ar mixtures are presented in Petersen, Hall, Kalitan, & Rickard (2004). The according correlations for acetylene and ethylene are shown in equation (2) and equation (3) respectively.

$$\tau_{C_2H_2} = 5.2 \times 10^{-14} [O_2]^{-1} \exp\left(\frac{79.5}{RT}\right) \quad (2)$$

$$\tau_{C_2H_4} = 3.3 \times 10^{-13} [C_2H_4]^{0.19} [O_2]^{-0.95} [Ar]^{0.04} \exp\left(\frac{26.6}{RT}\right) \quad (3)$$

While these simple equations can be used for a wide range of equivalence ratio  $\Phi$  values, for mixtures of different hydrocarbons additional shock tube experiments have to be performed. Higher hydrocarbons are usually more reactive than methane, therefore the ignition delay time is much lower. Even low concentrations of higher hydrocarbons (e.g. propane) in methane, lead to a drastic decrease of the ignition delay time. In Fig. 1 (a) the simulated ignition delay time for a mixture of fuel (15 wt-%), O<sub>2</sub> (30 wt-%), N<sub>2</sub> (55 wt-%) at 1 bar can be seen. The addition of 1 wt-% of propane to methane results in a decrease of the ignition delay time from 135.3 ms to 96.7 ms respectively (Fig. 1 (b)). Here the ignition delay time is defined as the time where  $\Delta T/\Delta t$  takes a maximum value.

**Fig. 1** Comparison of the simulated ignition delay of a mixture of

(a) 15 wt-% fuel (100 wt-% methane), 30 wt-% oxygen and 55 wt-% nitrogen and (b) 15 wt-% fuel (99 wt-% methane, 1 wt-% propane), 30 wt-% oxygen and 55 wt-% nitrogen

### Ignition Delay Time: Simulation

According to Joos (2006), using detailed chemical reaction mechanisms in perfectly stirred reactor simulations, a more general description of the ignition delay time can be achieved. These mechanisms are able to predict the ignition delay time for a wider range of conditions with good accuracy.

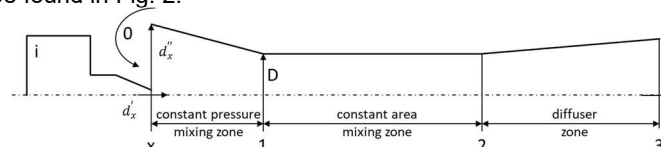
One of the most commonly used detailed reaction mechanism for the combustion of Methane is the GRI3.0 mechanism (Smith, et al.(2019)). It is a mechanism designed and optimized for modelling the combustion of natural gas, including NO formation and reburn chemistry. It consists of 53 species and 325 reactions.

An even more detailed reaction mechanism is the POLIMI C1-C3 HLT mechanism. It contains 107 species and 2642 reactions and is applicable for the pyrolysis, partial oxidation and combustion of hydrocarbon fuels up to 3 carbon atoms (POLIMI C1-C3 HLT (2019)).

## Materials & Methods

### Ejector Design

The ejector geometry is designed according to Keenan, Neumann, & Lustwerk (1950) as a function of initial primary (index i) and secondary gas (index 0) composition, temperature and pressure, the desired ratio of mass flow rates of secondary to primary stream  $\Omega$  and the nozzle diameter  $d_x'$ . The overall process is described by three subsequent process, namely constant pressure mixing, constant area mixing and diffusion. A detailed model description and how to use it can be found in Keenan, Neumann, & Lustwerk (1950). The schematic ejector geometry and important variables can be found in Fig. 2.

**Fig. 2** Ejector geometry and definition of important parameters

The mean residence time of the gas in the ejector can be calculated from the ejector volume  $V_{total}$  and the total volumetric gas flow  $\dot{V}_{total}$  using equation (4).

$$\tau = \frac{V_{total}}{\dot{V}_{total}} \quad (4)$$

Assuming perfect mixing in the ejector, the mean residence time  $\tau$  combined with ignition delay time  $\tau_{igni}$  for the exact conditions can be used to predict if ignition takes place in the ejector.

### Ignition delay

The ignition delay time is simulated for different species concentrations and temperatures at ambient pressure using the OpenFOAM® native solver *chemFoam*. It is a solver for chemistry problems, designed for use on single cell cases to provide comparison against other chemistry solvers, which use a single cell mesh.

Initial conditions, namely pressure  $p$  in Pa, temperature  $T$  in K, species concentrations  $Y_j$  in wt-% or mol-% and the constant property (volume or pressure), are provided in an *initialConditions* file. Thermo-physical properties, such as heat capacities  $c_p$  or the used equation of state, and reaction mechanism, which can be imported using the *chemkin-II* format, can be defined in the *thermophysicalProperties* file.

Output of the simulation are, amongst others,  $Y_j$ ,  $T$  and  $p$  over time. The possibility of using and comparing different reaction mechanisms and the possibility of automated simulation and evaluation, makes OpenFOAM® and the solver *chemFoam* a great tool to investigate ignition delay times and flammability limits under various conditions.

### CFD Simulation

To validate the assumptions of the 1D ejector design equations, two exemplary ejector geometries are simulated using Computational Fluid Dynamics (CFD). Simulations are carried out using the OpenFOAM®-solver *reactingFoam* and a 2D-axisymmetric approach and including gas reactions using different reaction mechanisms and without any reactions. Results are compared to the 1D ejector results. The influence of the different reaction mechanisms on the ejector behavior is shown

## Results & Discussion

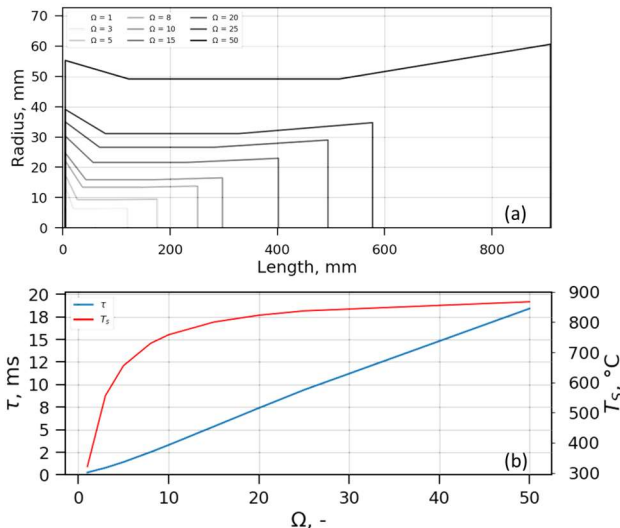
### Ejector Design

Conditions used in this study for designing the ejector are shown in Table 2. While the diameters  $d_x''$ ,  $d_2$  and  $d_3$  (see Fig. 2) can be calculated using the method described in Keenan, Neumann, & Lustwerk (1950), there are no correlations for the length of the different injector sections. In this study a value of  $L_j/D = 1.2$  was used for the constant pressure mixing length and  $L_j/D = 4$  was used for the constant area mixing and diffusion zone. Here  $L_j$  is the length of the respective zone and  $D$  is the diameter of the constant area mixing zone.

Resulting injector geometries are shown in Fig. 3 (a). Resulting mean residence times  $\tau$  and outlet temperatures  $T_3$  are shown in Fig. 3 (b). The outlet velocity  $v_3$ , outlet temperature  $T_3$  and mean residence time  $\tau$  for two exemplary ejectors are shown in Table 3.

**Table 2** Parameters used for the design of ejectors

parameter, dimension	symbol	value
ratio of specific heat air, -	$\gamma_{air}$	1.31
specific heat air, J/(kg K)	$c_{p,air}$	1155
ratio of specific heat methane, -	$\gamma_{CH_4}$	1.34
specific heat methane, J/(kg K)	$c_{p,CH_4}$	2221
ratio of specific heat flue gas, -	$\gamma_{fg}$	1.34
specific heat flue gas, J/(kg K)	$c_{p,fg}$	2000
stagnation pressure primary stream, bar	$p_i$	1.5
stagnation pressure secondary stream, bar	$p_0$	1.01325
stagnation pressure mixed stream, bar	$p_3$	1.01325
stagnation temperature primary stream, °C	$T_i$	20
stagnation temperature secondary stream, °C	$T_0$	900, 1200
nozzle diameter, mm	$d_x''$	2.5
mass flow ratio, -	$\Omega$	variable



**Fig. 3** (a) Ejector design, (b) mean residence time and outlet temperatures for different  $\Omega$  at  $T_0 = 900$  °C

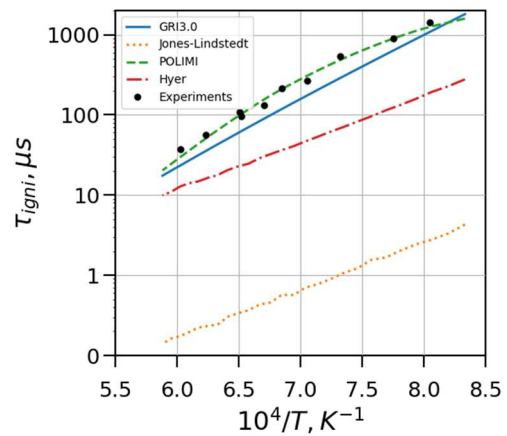
**Table 3** Important results of the 1D ejector design

$\Omega = 8$	$T_0 = 900$ °C	$T_0 = 1200$ °C
outlet velocity $v_3$ , m/s	65	67
outlet temperature $T_3$ , K	729	971
mean residence time $\tau$ , s	$2.92 \times 10^{-3}$	$2.74 \times 10^{-3}$

### Ignition Delay

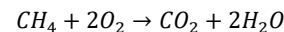
In CFD usually the use of detailed reaction mechanisms is not practicable because of the number of equations to solve, which leads to high simulation times. Thus usually skeletal mechanisms, containing a significant amount less reaction equations are used. In this study the Jones-Lindstedt (JL) skeletal mechanism (7 species, 4 reactions, Jones & Lindstedt (1988)) and the Hyer skeletal mechanism (8 species, 8 reactions, formulation according to Ahmed et al. (2014)) are used in addition to the detailed mechanisms.

The comparison of the simulated ignition delay time, using skeletal and detailed reaction mechanisms, to experimental ignition delay times (Petersen, et al. (2007)) for a methane/air mixture at 19.4 bar is shown in Fig. 4. One can see that the simulation gets more accurate when using more complex reaction mechanisms. The complexity increases from the Jones-Lindstedt (JL) mechanism, to the Hyer mechanism, the GRI3.0 mechanism and the POLIMI C1-C3 HLT mechanism. The ignition delay time is defined as the time where  $\Delta T/\Delta t$  takes a maximum value.



**Fig. 4** Comparison of the simulated ignition delay times of a methane/air mixture at 19.4 bar using the Jones-Lindstedt (JL), Hyer skeletal mechanism, the GRI3.0 mechanism and the POLIMI C1-C3 HLT mechanism to experimental results from Petersen, et al. (2007).

As stated before the ignition delay time and flammability limits are a function of the exact conditions (species concentration, temperature and pressure). In this study a number possible mixtures of fuel (99 wt-% CH<sub>4</sub>, 1wt-% C<sub>3</sub>H<sub>8</sub>) and air/exhaust gas (with different O<sub>2</sub> concentrations) at different initial temperatures are simulated to cover the whole range of operation conditions of the injector. The secondary stream is specified as a mixture of N<sub>2</sub>, O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O. Based on the difference between the reference O<sub>2</sub> concentration (23.135 wt-%) and cases initial O<sub>2</sub> concentration, the initial concentrations of the other species is changed. This is done according to the stoichiometry of complete methane combustion with oxygen:



In doing so, the ignition delay time and flammability limits of all possible  $\Omega$  and different compositions of the secondary gas are covered. All ignited cases at each temperature are then plotted in a ternary plot (e.g. Fig. 5).

Ignition is defined as a case where the following conditions are met:

- temperature increase  $\Delta T_{max} = T_{max} - T_0 \geq 250$  K
- ignition delay time  $\tau_{ign} \leq 0.2$  s
- the reaction has ended within the simulated time. The reaction is considered to be finished if the concentration of either O<sub>2</sub> or CH<sub>4</sub>  $\leq 1\%$  of the initial concentration, respectively.

The simulation of flammability limits and ignition delay times was carried out with settings according to Table 4 using the POLIMI reaction mechanism. Here  $\Delta$  is the step size for the respective property.

**Table 4** Simulation settings for the simulation of flammability limits and ignition delay times

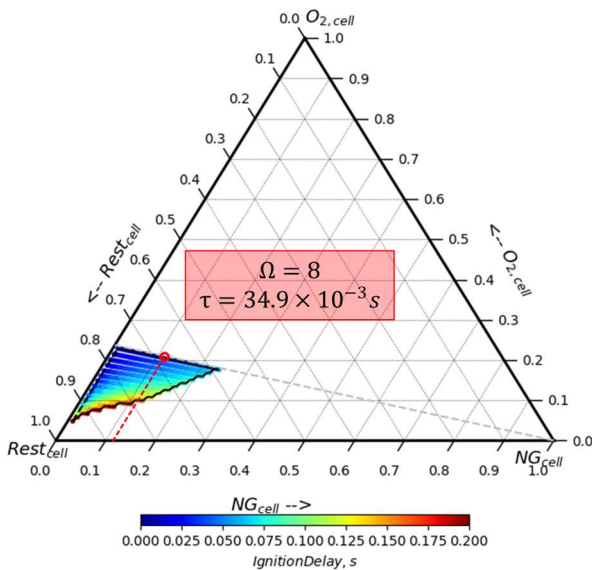
Property	min	max	$\Delta$
natural gas, wt-%	0	50	0.5
O <sub>2</sub> , wt-%	0.1350	23.135	1.15
T, K	1000	1300	20

Out of the 33936 simulations 3381 cases have ignited. Only eight simulated cases have ignited for an initial temperature of 1000 K. It is safe to assume that no ignition takes place below this temperature. Ignited cases for an initial temperature of 1240 K are shown in Fig. 5. The color indicates the ignition delay time for the respective mixture. The dashed grey line represents all possible mixtures of natural gas (NG) and air, thus also represents the ratio of mass flow rates of secondary to primary stream  $\Omega$ . This ration can be calculated out of the desired natural gas concentration according to equation (5), where [NG] is the concentration of natural gas.

$$\Omega = \frac{1 - [\text{NG}]}{[\text{NG}]} \quad (5)$$

Each ejector design can be checked for possible ignition in the ejector, when assuming perfect mixing and using equation (5), the mean residence time in the ejector  $\tau$ , the outlet temperature  $T_3$  and the according ternary plot.

T = 1240.0K



**Fig. 5** Ternary plot of natural gas (NG) oxygen (O<sub>2</sub>) and air/exhaust gas (Rest) including region of flammability and ignition delay times. An exemplary designed ejector is marked with a red circle.

For the exemplary ejector with  $T_0 = 900 \text{ °C}$  the predicted outlet temperature  $T_3$  is 1002.1 K (729 °C). For this temperature and  $\Omega$  no ignition is achieved in the ignition delay study.

For a higher temperature of the secondary gas stream of  $T_0 = 1200 \text{ °C}$  the predicted outlet temperature  $T_3$  is 1244.4 K (971 °C). At this temperature and for a gas concentration of 11 wt-% ( $\Omega = 8$ ) ignition can be achieved, as indicated in Fig. 5. But when comparing the ignition delay time

$\tau_{igni} = 34.9 \times 10^{-3} \text{ s}$  with the predicted mean residence time  $\tau = 2.74 \times 10^{-3} \text{ s}$  it can be seen that, despite the point lying within the flammability limits, no ignition is achieved in the ejector.

## CFD

CFD simulations have been carried out for conditions shown in Table 2 using ejectors designed for  $\Omega = 8$ . Gas phase reactions are considered using the detailed GRI 3.0 and the Hyer skeletal mechanism. The gaseous fuel consists of 99 wt-% methane and 1 wt-% propane. The secondary gas stream is air. Simulations are evaluated regarding the ratio of mass flow rates of secondary to primary stream  $\Omega$ , the temperature  $T_3$  and velocity  $v_3$  at the ejector outlet and the mean residence time of both, reacting and non-reacting flows. Also the presence/absence of reaction in the ejector is evaluated for the different reaction mechanisms.

Results for  $T_0 = 900 \text{ °C}$  and  $T_0 = 1200 \text{ °C}$  for a non-reacting flow are shown in Table 5. While  $\Omega$ ,  $T_3$  and  $\tau$  are in reasonable good agreement from 1D (Table 3) to CFD (Table 5) simulation (within 15 %), the outlet velocity  $v_3$  does deviate by > 30 %. One reason for that is the error in the prediction of the outlet temperature. Applying the CFD-simulated  $T_3$  to the 1D simulation reduces the deviation to < 15 % from 1D to CFD simulation for the outlet velocity  $v_3$ .

**Table 5** CFD results for two different ejector designs. Reactions are not included.

no reactions	$T_0 = 900 \text{ °C}$	$T_0 = 1200 \text{ °C}$
mass flow ratio $\Omega$ , -	7.62	7.8
outlet velocity $v_3$ , m/s	48.8	50.9
outlet temperature $T_3$ , °C	663.7	874.5
mean residence time $\tau$ , s	$3.4 \times 10^{-3}$	$3.3 \times 10^{-3}$

When considering gas phase reactions the results deviate significantly from 1D to CFD simulation. As indicated by the outlet temperature  $T_3$  shown in Table 6, the fuel/gas mixture is igniting within the ejector tube. This shows that the assumption of perfectly mixed gases is not valid. When the secondary gas is sucked in, the local conditions (temperatures, gas composition) differ significantly from the average values. Thus in such mixing zones the ignition conditions are met and ignition is possible at very low ignition delay times. Using a skeletal reaction mechanism, the ignition delay time is clearly under predicted (Fig. 4, Hyer and Jones-Lindstedt), compared to the more accurate detailed mechanism. This leads to even higher fuel conversion and outlet temperatures  $T_3$ .

Results shown in Table 6 also reveal that ignition in the ejector has significant influence on the mass flow ratio  $\Omega$ . Using the detailed reaction mechanism the simulated  $\Omega$  differs by 41 % compared to the design case. A difference of 94 % is found when using the skeletal Hyer reaction mechanism. As the GRI 3.0 mechanism is considered to be more accurate, the CFD results using the detailed mechanism are considered to be the most realistic amongst the tested simulation methods.

**Table 6** CFD results for two different reaction mechanisms.

$T_0 = 900 \text{ °C}$	Hyer	GRI 3.0
mass flow ratio $\Omega$ , -	4.12	5.67
outlet velocity $v_3$ , m/s	60.82	53.2
outlet temperature $T_3$ , °C	1328.25	988.7
mean residence time $\tau$ , s	$3.15 \times 10^{-3}$	$3.45 \times 10^{-3}$



### Summary & Outlook

The model equations presented in Keenan, Neumann, & Lustwerk (1950) have been successfully applied to design ejectors for gaseous fuels at low pressure ratios  $P^i/p_0$ . The 1D method proves to be in good agreement with CFD simulations (deviations of < 15 %, except for the outlet velocity  $v_3$ ), if no ignition takes place in the ejector.

A detailed investigation on the ignition delay time and flammability limits of gaseous fuels (methane, methane/propane mixture) under various conditions was carried out. Results have been used to try to predict if ignition takes place in the designed ejectors. As shown using CFD simulation and a detailed reaction mechanism (GRI 3.0), the assumption of perfect mixing in the ejector tube is not correct. In certain regions of incomplete mixing ignition conditions are met. This is true even if the predicted residence time  $\tau$  (e.g.  $3.4 \times 10^{-3}$  s for  $\Omega = 8$ ) is approximately an order of magnitude lower than the ignition delay time  $\tau_{igni}$  (e.g.  $34.9 \times 10^{-3}$  s) using averaged gas properties.

It was also shown that, in order to predict an accurate ejector behavior, it is mandatory to correctly consider ignition delay. Thus the use of detailed reaction mechanisms is recommended. Also an experimental validation of the simulated ejector using gaseous fuels under ignition condition is highly recommended.

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