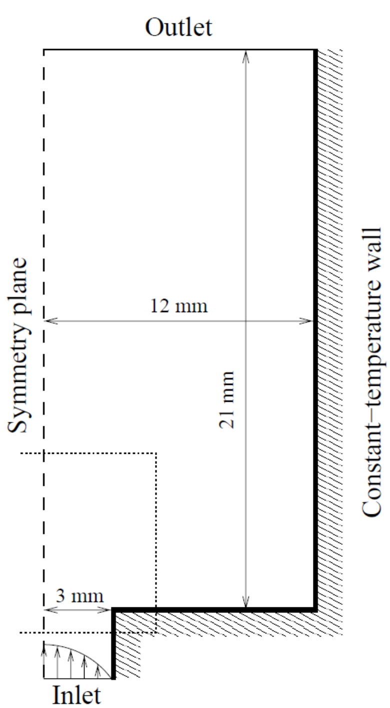
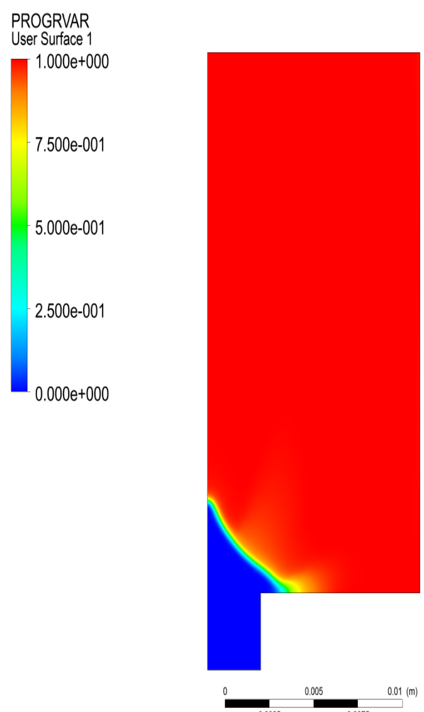
Implementing the Flamelet Generated Manifolds technique into Comsol to simulate reacting flows

In this BEP end project proposal the goal is to implement the technique of Flamelet Generated Manifolds (FGM) into the flow solver Comsol. The method of FGM is developed at TU/e to reduce the complexity of the chemistry in numercal simulations of combustion. It also removes the stiffness of intermediate reactions that can be very fast. At the same time the accuracy of the simulation is remained. This makes it possible to predict emissions of e.g. pollutants with a high accuracy. This method is now being introduced also for turbulent flow conditions. The method was first implemented in numerical codes that were developed in house. More and more the method is introduced in commercial codes like Fluent, CFX, OpenFOAM etc.. This to simulate large scale combustion systems like gas-turbines, engines, furnaces etc..However in order to check implementations a simple test is necessary. For doing this it is suggested to simulate the so-called “flame in a box” which is 2D and laminar. Furthermore both steady as well as unsteady solutions can be used. This also holds for compressible as well as incompressible versions. Additionally we have produced accurate solutions for this flame with a direct numerical simulation with detailed chemisty and complex transport. Also experiments have been carried out for this flame. A simple general framework to do produce a reference case would be to use the Comsol multiphysics program to simulate Navier-Stokes equations; which is the main task of this “research”.

The geometry of the “flame in a box” is displayed in the figure at the left. Premixed mixture flows from the bottom upwards. At a certain position it stabilizes. This cas be seen in the right picture, which is the progress variable (a measure for temperature if you want).





Info: R.J.M. Bastiaans, Gemini N 1.46 r.j.m.bastiaans@tue.nl

Implementing the Filtered Flamelet Generated Manifolds technique into Comsol to simulate reacting flows at relatively low resolution

In this BEP end project proposal the goal is to implement the technique of Filtered Flamelet Generated Manifolds (FGM) into the flow solver Comsol. The method of FGM is developed at TU/e to reduce the complexity of the chemistry in numercal simulations of combustion. It also removes the stiffness of intermediate reactions that can be very fast. At the same time the accuracy of the simulation is remained. This makes it possible to predict emissions of e.g. pollutants with a high accuracy. This method is now being introduced also for turbulent flow conditions. The method was first implemented in numerical codes that were developed in house. More and more the method is introduced in commercial codes like Fluent, CFX, OpenFOAM etc.. This to simulate large scale combustion systems like gas-turbines, engines, furnaces etc.. Because often the combustion fronts are thinner then the smallest eddy size in the flow it is possible to resolve the flame with a minimum number of grid-points. This can be done by filtering the manifold to be resolvable on a given computational grid. A first test to validate this concept is to do this with a cold reaction in a whirling flow. In this case there is no back-coupling of the reaction to the flow. If the concept would not work for this case, it would certainly not work for expanding reacting laminar and turbulent cases. The starting point is a 2D rotating flow on a periodic domain in Comsol as displayed below in figure 1. On top of that we put a scalar field of a combustion progress variable that has values of zero in the lower half, and 1 in the upper half increasing from 0 to 1 with a certain thickness with a hyperbolic tangent function mimicking a flame front. This progress variable has a source term which enables it to propagate (from top to bottom). On a fine 1D grid we can retrieve the propagation velocity. Now we can access the regime diagram with adjusting firstly the ratio of burning velocity and initial flow amplitude and secondly the size of the initial vortices compared to the thickness of propagation region. We can do a study for different cases by decreasing the numercal resolution and increasing the size of the source term filter.

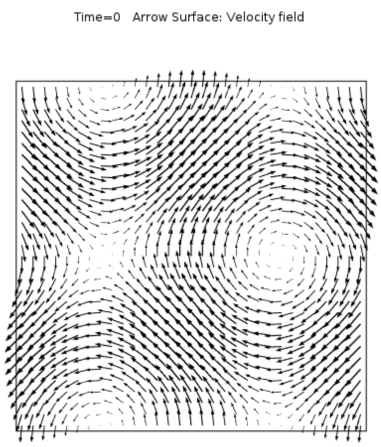


Fig. 1. The initial flow

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MILD Combustion Simulation using Fluent

In order to increase the efficiency of a combustion system, it is desirable to recover the heat that goes off with the exhaust gases. However, as the waste heat is recovered and the peak temperature of the combustion system increases, the level of Nitric Oxide (NO_x) emission, which is harmful to human health, also increases. In order to reduce the NO_x production without sacrificing the gain from heat recovery, the oxidizer and/or the fuel might also be diluted with the exhaust products. When the level of dilution and the heating of the reactants are so high that autoignition takes place, the system is in the MILD combustion regime. In MILD combustion, the efficiency of the system is increased without the penalty of increased NO_x emissions, which makes it a promising combustion technology.

In Combustion Technology Group of TU/e, we simulate turbulent MILD combustion in order to better understand the physical mechanisms (and interactions among them) like turbulence, chemistry and diffusion in MILD conditions. In simulations, we use codes developed in our group. However, we also desire to use commercial code ANSYS Fluent to simulate MILD combustion. Although this aim is achieved through a BEP Project completed in the second quarter, simulation results are far from matching the results of jet in hot coflow (JHC) experiments of Delft University of Technology. Therefore, the task of the BEP student will be the improvement of the developed model and trying to predict the experimental results sufficiently. Some of the improvements might be listed as; implementation of real experimental profile as boundary condition, fine tuning of turbulence parameters, implementation of a better molecular transport model and most importantly the prediction of NO_x emissions.

In the end, student will be familiar with combustion and related physical phenomena like turbulence, chemistry and diffusion, computational fluid dynamics, ANSYS Fluent package and will probably improve the skills in MATLAB.

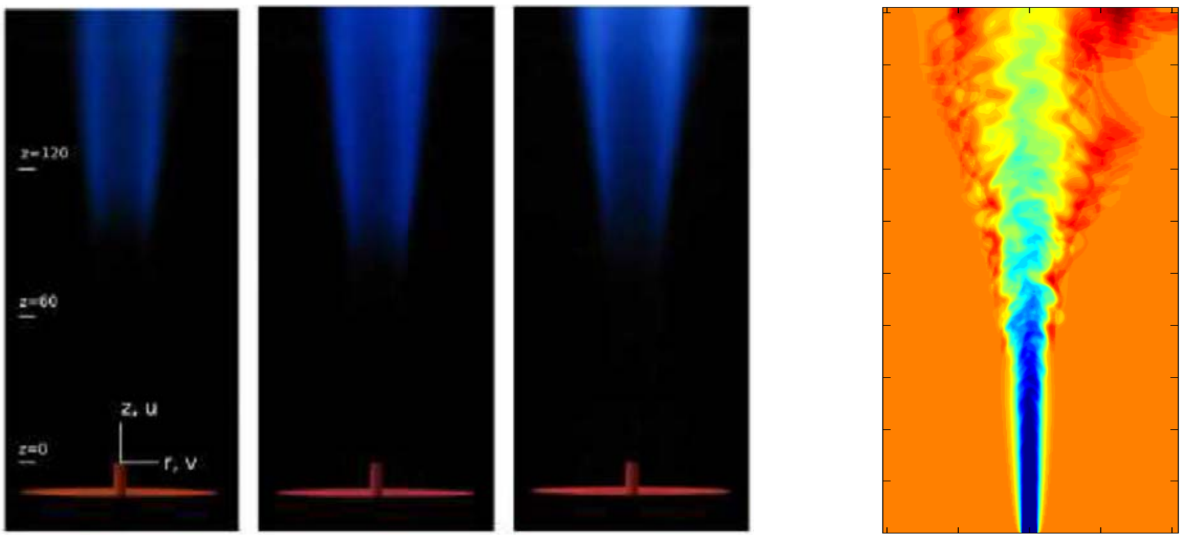

Figure: Image from Delft Jet in a Hot Coflow Experiment and a Contour Plot of Temperature from a Simulation Conducted in Our Group

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Ebrahim Abtahizadeh, Gemini Noord 1.41, e.abtahizadeh@tue.nl

BEP Assignment: Future energy flows.

Energy demands in The Netherlands are changing. More and more we see a shift towards pollution free transforming of energy. Energy scenarios are published all around to forecast what our future could look like. Alliander N.V. (The largest grid operator in The Netherlands) wants to know what this energy future looks like in order to make the right considerations when investing in the energy distribution grid.

The assignment will first focus on extracting different energy scenarios from literature and ordering them in a logical way. After this, you will make your own forecast in what the energy future would look like and what this would mean for the average Dutch household. With energy calculations you should be able to answer the simple questions about our energy usage, such as: Will electric cars reduce our energy consumption? Would we still need a HR++ boiler to heat our rooms? Will solar panels save the world? The central question is: How can humankind use energy in the best possible way?

Goals of the assignment:

- Make an inventory of different energy scenario's
- Logical ordering of energy scenario's
- Prioritizing and molding into a single scenario for The Netherlands
- With this scenario, calculate the energy flows of a Dutch household

So if you want an assignment that challenges you to think about our future and use basic energy flow calculations to make it as realistic as possible, don't hesitate and sign up!

Contact details:
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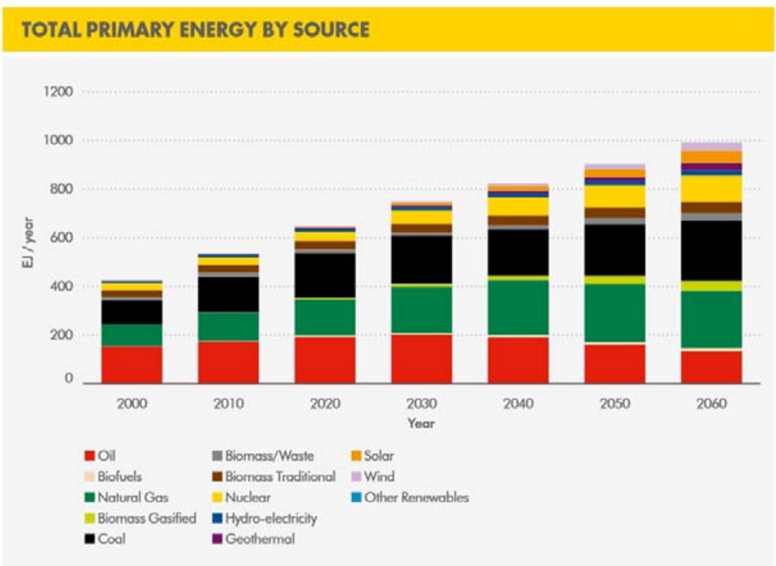
E-mail: B.F.W.Vermeltfoort@tue.nl



Total primary energy by source, "New Lens Scenario", Shell 2013.

BEP assignment

At the combustion group we do research on future combustion concepts for HD diesel engines. These concepts heavily rely on auto-ignition. Traditionally the 'ignition quality' of fuels is specified by the so-called ON (Octane Number). Pump fuels typically have an octane number of 95 which means that for a very specific test (Octane test) it behaves like a mixture of 95% octane and 5% n-heptane.

We now have every reason to belief that this Octane number is not enough to specify fuels for the new combustion concepts. Currently we are planning experiments with two different fuels at some pre-defined engine loads (specific RPM and Power setpoinst) on our research engine. Fuel 1 consist of 70% i-octane and 30% n-heptane (per definition an exact ON70 fuel) and Fuel 2. A blend of butanol/i-octane/n-heptane. Both blends have an ON70 according to the official Octane test. In this assignment we want to study the ignition behavior of both blends by simulation of Homogeneous Reactors (HR). We want to apply detailed chemical mechanism that are available to compute the auto-ignition and of both fuels for relevant experimental conditions.

The assignment

- Determine the relevant conditions for the HR, meaning the right temperature and pressure and concentrations before ignition.
- Compute the ignition delay for both fuels at these conditions using our in-house code.
- Determine the sensitivity of the ignition delay of Fuel 2 with respect to small variations of butanol and i-octane.
- Compare to the experimental findings.

Contact

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GN 1.42

ENABLING ENGINE KNOCK MONITORING FOR THE NEW VOLVO T5 ENGINE SET-UP

Earliest starting date: Startdate SEP assignment Jeffrey van den Broek

Currently, at the TU/e a new Volvo Turbocharged SI (Spark Ignition) engine set-up is built in engine cell 2 intended for research on inter alia, alternative fuels, i.e. E85, CyclOx, and other fuels like Tall oil derived naphtha like fuels. These fuels are characterized by their higher ON (Octane Number) with respect to EURO95 gasoline. The benefit of a higher ON is that a higher compression ratio and therefore higher thermal efficiencies can be achieved. During experimental research, limits for engine knock will be investigated which requires intensive engine knock monitoring to prevent harming the engine. This can be done by e.g. connecting knock sensors to the microphone input of a laptop and recording an audiogram.

Preliminary research was performed by a Fontys Applied Sciences graduate student (Jeffrey van den Broek) and experiments were performed regarding the position of the additional knock sensors. Not all the goals of the initial assignment were achieved (e.g. goal 3.) during the preliminary research and further research is necessary to ultimately achieve the goals.

The goals of this internship assignment are to:

1. Perform a literature study on the engine knock phenomenon.
   - What exactly is engine knock?
   - How can engine knock be identified?
   - In which frequency range does engine knock occur? Which engine parameters influence engine knock and determine the frequency for which it occurs?
   - Which methods and measurement tools (e.g. microphones, accelerometers, and pressure sensors) can be used to monitor knock onset and knock intensity as accurate as possible?
   - How could the system be calibrated?

2. Write a detailed plan of approach

3. Design and build, with support of an electrical technician, a system to record, plot and analyze engine knock.

4. Write a report of your work and conclude it with a presentation.

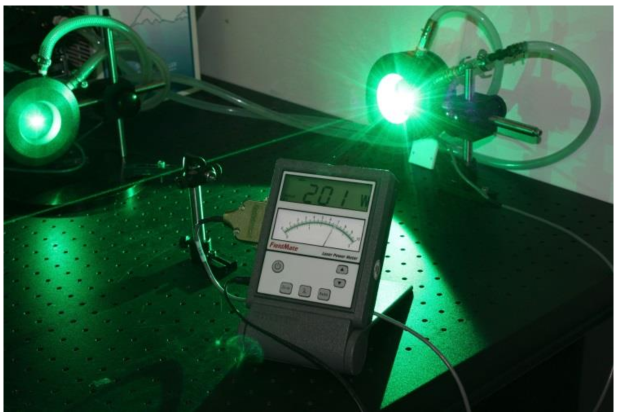
The focus in this assignment will be on goal 3.

Direct supervisor:	Ir. R. Dijkstra
Indirect supervisor:	Prof. P. de Goey, Dr. M. Boot
Electrical technician:	W.J. Loor

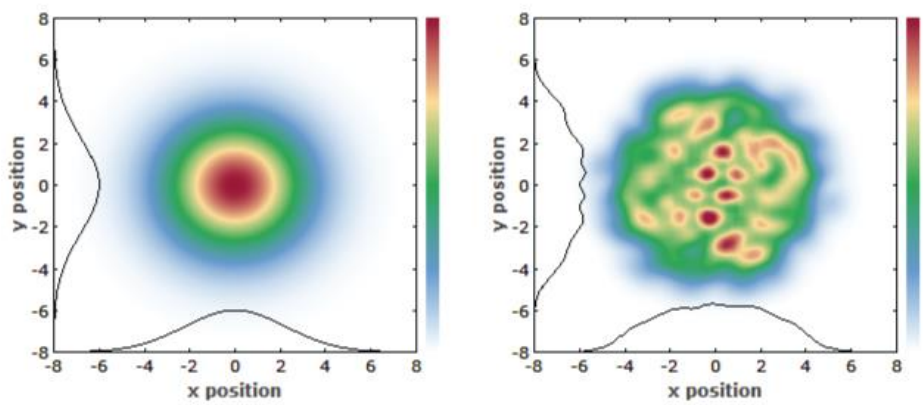
Bachelor End Project

The Quantification of Laser Sheets

From the combustion process to the atmospheric droplets, laser diagnostics plays an important part in the imaging of physical processes. The use of high powered lasers, usually Nd:YAG lasers, has become commonplace at the frontier of new research.



However, the profiles of the laser spots and laser sheets created using YAG lasers are often not a block or even a Gaussian one! Even though the profiling of such lasers are of high importance on the data processing and results, they are often investigated by eye and crudely approximated. Someone has to change this, and that someone is you!



Laser profiles can be a simple Gaussian (left) or a much more complex pattern (right). The shape of the profile will determine a significant part of the outcome of an experiment.

The goal of this project is to create 2D intensity profiles of the UV laser spots and sheets created by a Nd:YAG pulse laser. Optimization of the thickness of laser sheets without introducing diffraction, and the uniformity of laser spots, will be part of the research.

Contacts:

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Dennis van der Voort	d.d.v.d.voort@tue.nl	Cascade 2.25

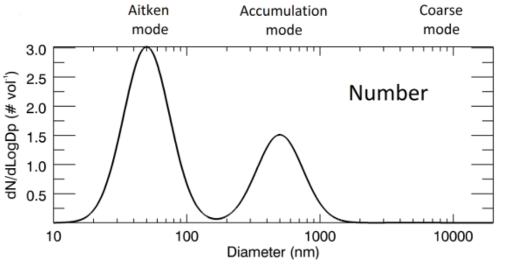
BEP opdracht

Analyse van roetdeeltjes-grootteverdeling van GTL en diesel brandstoffen

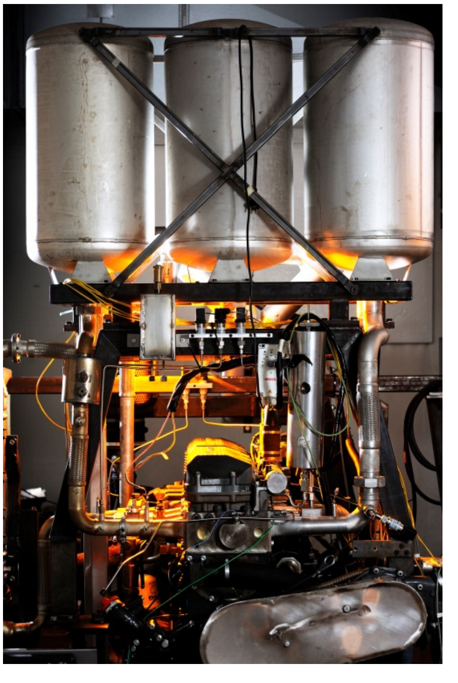
Achtergrond

De uitstoot van schadelijke emissies is de laatste decennia drastisch afgenomen. Met name de roetuitstoot is terug gedrongen van de zwarte rook uit de uitlaat naar geen visueel zichtbaar roet. Maar dit betekent nog niet dat er helemaal geen roetuitstoot meer is. De roetdeeltjes zijn kleiner geworden waardoor ze minder zichtbaar zijn maar juist deze kleine deeltjes zouden erg schadelijk zijn voor de gezondheid.

Om uit te zoeken wat de invloed is van verschillende brandstoffen zijn er metingen uitgevoerd met een instrument dat de deeltjesgrootteverdeling kan meten. Deze resultaten zullen aandachtig geanalyseerd moeten worden om verbanden te kunnen leggen tussen brandstofeigenschappen en de deeltjesgrootte.



Roetdeeltjesgrootte verdeling



Testopstelling: 12,6L motor

Opdracht

- Literatuurstudie over roetdeeltjesgrootteverdeling
- Metingen analyseren van deeltjesgrootte meter
- Resultaten verwerken en verbanden leggen
- Vergelijk diesel met GTL brandstoffen
- Rapporteer je bevindingen

Contact informatie

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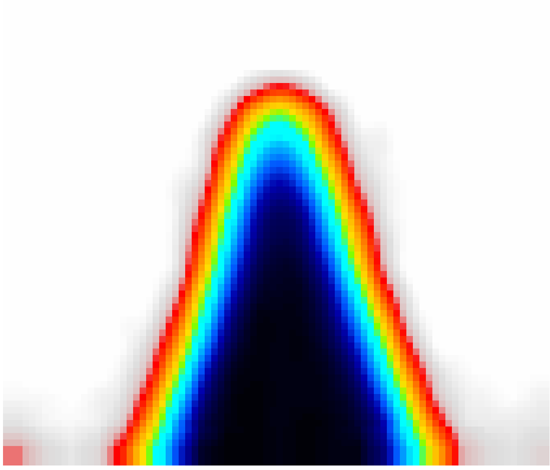
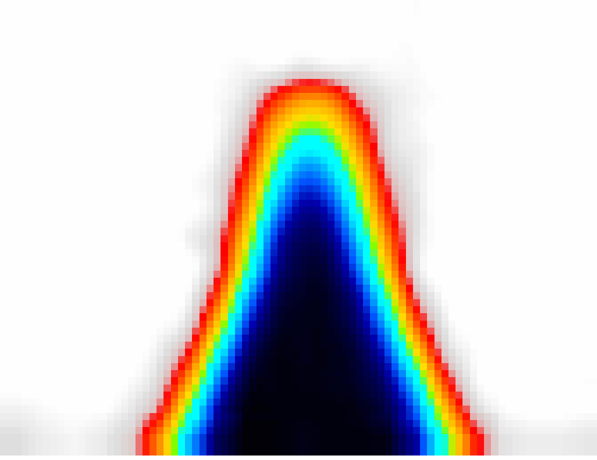
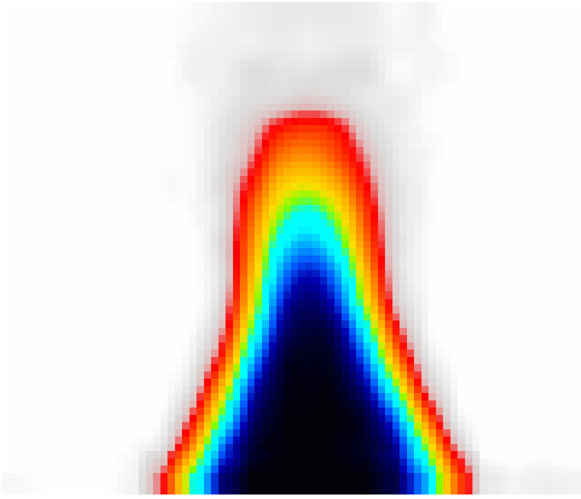


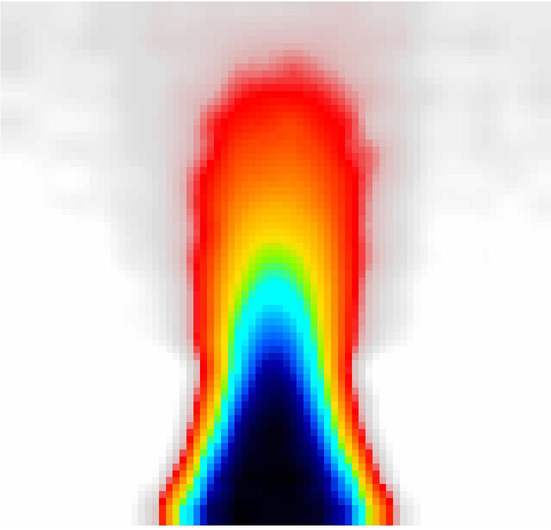
CH4, S_L = 10 cm/s



0.2H2 + 0.8CH4, S_L = 10 cm/s



0.4H2 + 0.6CH4, S_L = 10 cm/s



0.6H2 + 0.4CH4, S_L = 7 cm/s

De verbranding van waterstof-methaan mengsels krijgt momenteel veel aandacht vanwege de plannen om aardgas te mengen met waterstof uit duurzame bronnen (vergassing van biomassa, elektrolyse met zonne- en windenergie). Recentelijk hebben we zeer nauwkeurige metingen verricht aan Bunsen vlammen van methaan-waterstof mengsels. Door de hoge diffusiviteit van waterstof gebeuren er bijzondere dingen. Bij hoge concentraties waterstof lijkt de vlamtip open te breken! (zie temperatuur metingen hierboven)

Om dit verschijnsel beter te kunnen begrijpen, willen we deze vlammen numeriek modelleren. Het doel van deze BEP opdracht is om deze vlammen te simuleren en de resultaten te vergelijken met de metingen.

Contact: Jeroen van Oijen (j.a.v.oijen@tue.nl)

Sensitivity Study of Spray Models in STAR-CD

Spray formation is a significant phenomenon in diesel combustion. It is essential to predict mixture formation and emissions accurately. However, to comprehend the physical processes occurring during spray formation is not easy.

The commercial CFD tool Star-CD is used for the simulations. Various sub-models (Table 1) can be chosen in Star-CD to model nozzle flow, atomization and droplet break-up processes.

Table 1: *Available sub-models*

Nozzle Flow	Droplet Breakup	Atomization
Effective model	Reitz and Diwakar model	Huh's model
MPI model	Pilch and Erdman model	Reitz-Diwakar model
Modified MPI model (MPI2)	Hsiang and Faeth model	MPI model
		Modified MPI model

The aim of the project is to find the optimum combination of the sub-models by making a sensitivity study. Well-defined operating conditions exist and the results can be compared to the experimental data. Spray penetration, liquid length results and mixture formation profiles will be utilized to find the optimum setting.

Contact:

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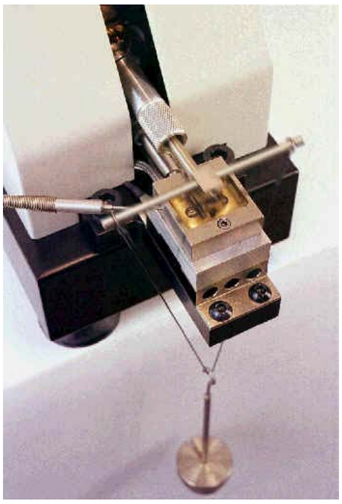
Bart Somers (l.m.t.somers@tue.nl, tel: 2107)

BEP opdracht: Een meetmethode voor de 'smeerbaarheid' van brandstoffen

Periode: kwartiel 4 & interim, studiejaar 2012-2013
Begeleiders: · Harry van Leeuwen en Michael Boot

Inleiding



In de verbrandingsmotor zijn er verschillende bewegende onderdelen die met behulp van de brandstof zelf worden gesmeerd. Gebleken is dat diesel als brandstof veel beter smeert dan benzine, en dat ook de gebruikte additieven in de brandstof van groot belang zijn. Deze smerende werking wordt in de literatuur wel aangeduid als 'lubricity' (smeerbaarheid). 'Lubricity' zou kunnen worden omschreven als de eigenschap om onder toepassingscondities te zorgen voor een lagere wrijving en een lagere slijtage dan een vloeistof van gelijke dynamische viscositeit realiseert. Dit lijkt op het eerste gezicht raar, maar is te begrijpen als de werkelijke contactsituatie erin betrokken wordt. Als deze eigenschap relevant wordt, is het contact zó slecht gesmeerd dat er geen volledige scheiding van de bewegende onderdelen uit de loopvlakbeweging kan worden verkregen. Dan glijden ze dus over elkaar, waarbij er tevens op microschaal contact is. De gevolgen hiervan zijn catastrofaal, tenzij er zich chemisch of fysisch gebonden lagen met lage schuifspanning vastzetten op de loopvlakken, ter bescherming en ter verlaging van de wrijving.

Opdracht

1. Inwerken in de probleemstelling door bronnenstudie, beginnende met de literatuur in de referentielijst, waaruit blijkt dat de theorie goed is begrepen. Het rapport van Meesters [1] maakt een snelle start mogelijk. De resultaten van de literatuurstudie worden ook in beknopte vorm opgenomen in het verslag.
2. Beantwoord in specifieke en gedetailleerde bewoordingen de vraag, wat smeerbaarheid is.
3. Geef een eigen en tevens kritische reflectie op bestaande meetmethoden, en kom op grond daarvan met een voorstel voor een methode. Dit mag ook uitdrukkelijk een niet bestaande methode zijn.
4. Vervolgens wordt daarbij een tribometer gezocht, die het meest geëigend is en die beschikbaar is, waarmee lubricitymetingen worden gedaan aan een referentie dieselbrandstof en een eigen diesel brandstof. Stel in overleg met de begeleiders hiervoor de meetcondities en een meetplan op.
5. Schrijf een beknopt verslag, waarin het voorgaande is beschreven.
6. Houd een mondelinge presentatie over dit werk.

Referenties

[1] Meesters, C.J.M., 2012, "Lubricity", *Intern Rapport TU/e,* TU Eindhoven, Netherlands, 71 pp.

[2] Lacey, P.I. and Westbrook, S.R., 1995, "Effect of fuel composition and prestressing on lubricity", U.S. Army TARDEC, Fort Belvoir, Virginia, USA, Contract No. DAAK70-92-C-0059

[3] Wei, D. P. , Spikes, H. A., and Korcek, S., 1999, "The Lubricity of Gasoline", *Tribology Transactions*, Vol. 42, No. 4, pp. 813-823, DOI:10.1080/10402009908982288

[4] Masuch, K., Fatemi, A., Murrenhoff, H., and Leonhard, K., 2011, "A COSMO-RS based QSPR model for the lubricity of biodiesel and petrodiesel components", *Lubrication Science*, Vol. 23, No. 6, pp. 249-262

[5] Barunovic, R., Haas, V., Langlade, C., and Krill III, C.E., 2012, "Sliding wear of 100Cr6 in a diesel-lubricated flat-flat contact under realistic loads", *Tribology International*, Vol. 53, pp. 1-11

Title: Surface temperature measurement using Thermographic phosphor technique

Supervisors: Mayuri Goswami, Nico Dam, Philip de Goey

Description: Thermographic phosphor technique has recently emerged as a potential temperature measurement technique. Thermographic phosphor is a phosphorescent material that has temperature dependent emission. A tripled Nd:YAG laser (355 nm) is used as excitation source and the emission intensity is measured with an ICCD camera through a custom-made stereoscope. The stereoscope makes two images of the same object which is further filtered with two band pass filters of specific wavelength bands. The ratio of intensities from both images is directly related to the temperature of the surface. This is termed as the spectral ratio method. The main goal of the project is to measure temperature of a flat brass plate coated with the phosphor, first using thermocouples and then produce an accurate calibration of the thermographic phosphor measurements.

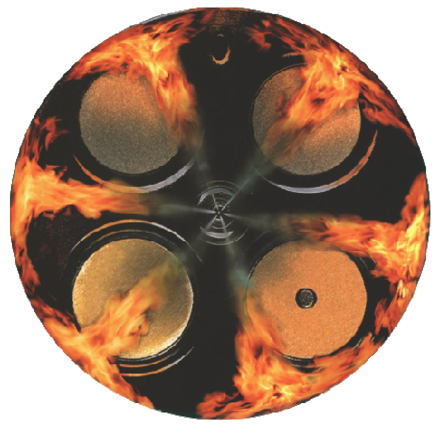
Picture: A ZnO:Zn phosphor coated plate when excited by 355 nm YAG laser in presence of a methane/air flame.

Bachelor Eind Project

Relatie bepalen tussen roetdeeltjes in en na de verbranding

Achtergrond

Met name dieselmotoren zijn de laatste decennia vele malen schoner geworden. De NO_x- en roetuitstoot zijn drastisch gedaald waardoor de grootte van de roetdeeltjes belangrijker wordt. Steeds vaker wordt de fijnstof in de lucht gekoppeld aan de gezondheid van de mens. Roetuitstoot is een belangrijke bron van deze fijnstof.



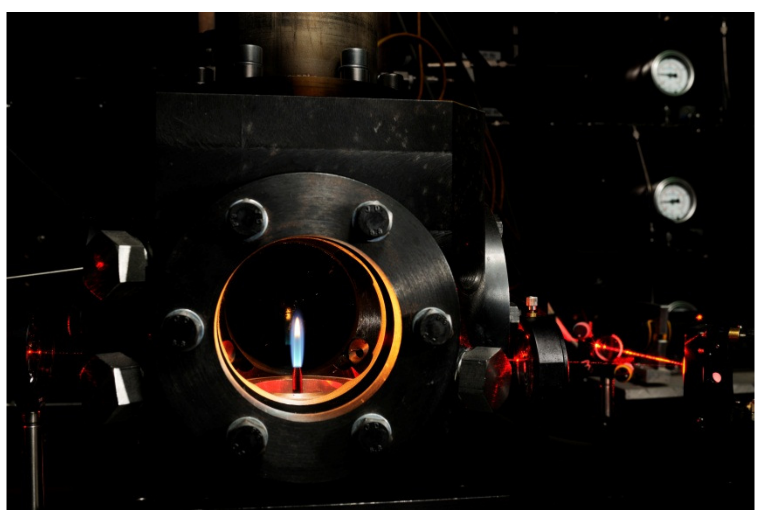
Verbrandende spray

Op dit moment is er weinig bekend over de relatie tussen roetdeeltjes tijdens de verbranding (in de vlam) en na de verbranding (in de uitlaat). Zijn deze evenredig aan elkaar gekoppeld of vinden er tussendoor nog andere reacties plaats die nog onbekend zijn? En zo ja, welke?

In deze BEP opdracht is het de bedoeling om te onderzoeken of er een relatie is tussen de deeltjes grootte in de vlam en buiten de vlam. Hiervoor moet gekeken worden naar een geschikte meetmethode om daarmee ook experimenten uit te kunnen voeren.

Doelen

- Korte literatuurstudie over roetdeeltjes
- Meetmethode bepalen
- Metingen uitvoeren
- Resultaten analyseren
- Bevindingen rapporteren



Meet opstelling: hoge druk brander

Meer informatie?

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BEP Assignment
R&D of flame sensor for variable fuel gas at domestic appliances

Supervision: dr. ir. Viktor Kornilov (GEM.N 1.44)

Problem description

The expected in the nearest future diversification of sources of fuel gas will lead to introduction of hydrogen, CO and heavier then methane hydrocarbons into the natural gas grid over the Europe. It is foreseen that the variation of the gas composition will be not only by regions but also in time at fixed location.

Conventional domestic appliances (heating boilers, a kitchen stove, driers, CHP systems, etc.) have to be adjusted properly to adapt the variability of the fuel quality. Additions of hydrogen, CO, N_2 heavy hydrocarbons change the mixture calorific value, burning velocity, flame temperature and stabilization behavior dramatically. As a result, malfunctioning of heating appliances is possible which, in severe case, may even cause a damage of equipment.

source: robogas.nl

Project

Team of company ATAG (leading organization), TU/e and Kiwa initiated a project aiming to find possible measures to adapt burners typically used in kitchen stove for new fuels. Dutch government (Agentschap.nl) has supported this initiative. The contribution of TU/e which also constitutes the contents of the present project consists of two parts:

- Investigation of practically relevant consequences of fuel variability for the functionality of above mentioned type of burner;
- Proposition, study (including experiments) and evaluation of technical applicability of different sensing methods to detect the gas/flame variability in time.

Work assignment

The work will include:

- design and construction of laboratory setup based on the industrial burner;
- study of different techniques of flame/gas sensing;
- experimental evaluation of applicability of different sensing methods to detect the fuel gas variation;

- elaboration of recommendations for the practical solution of the gas variability problem in kitchen stove burner.

The research is practically oriented; however it will also address the broad range of fundamental aspects of combustion physics and measurements techniques.
It is expected, that the student working on the project will be the principal executer of the TU/e part of work foreseen within this project.
The work will be conducted in a close cooperation with industrial partners.