Influence of multicomponent fuel composition on ignition and combustion of diesel sprays

4th Two-day Meeting on Internal Combustion Engine Simulations Using OpenFOAM® Technology

TECHNISCHE UNIVERSITÄT DARMSTADT

STFS

LED Low Emission Design

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Bundesministerium für Wirtschaft und Energie
aufgrund eines Beschlusses des Deutschen Bundestages

STFS

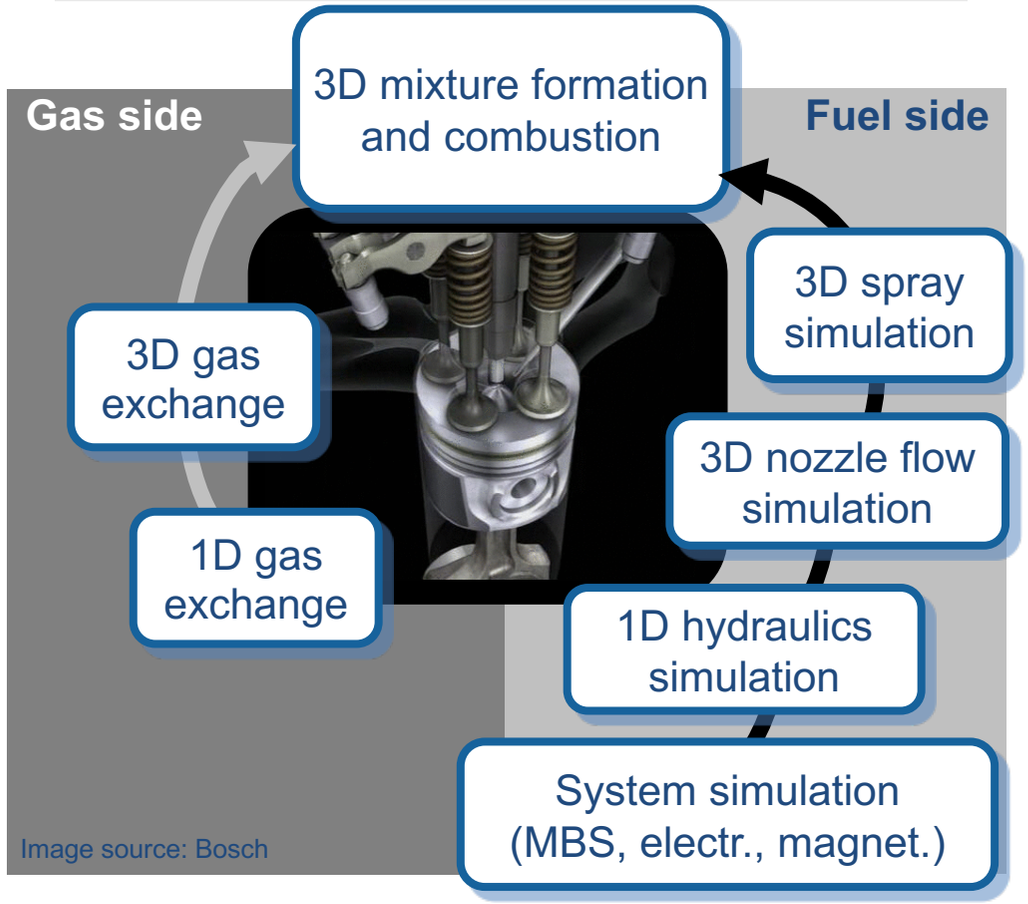
HSM

LTT ERLANGEN

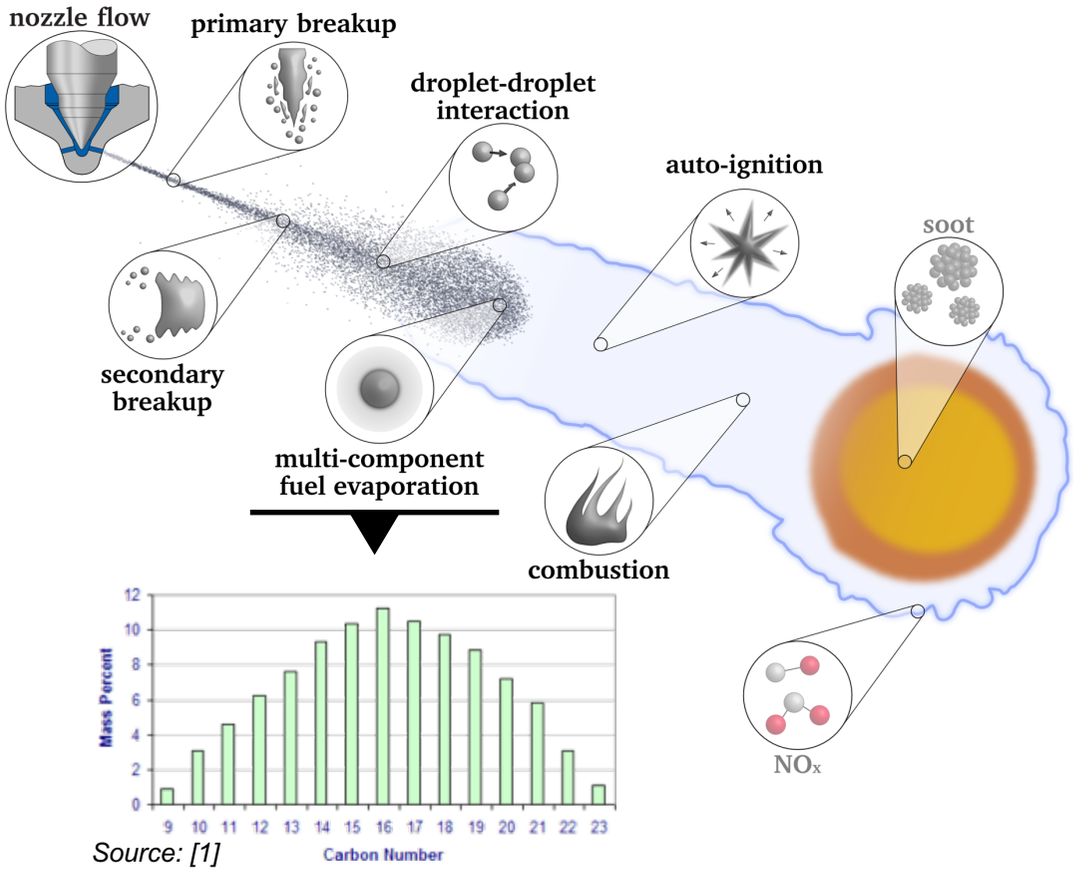
RECK Modeling Group

Motivation

The entire diesel process



Zoom into diesel spray cause effect chain



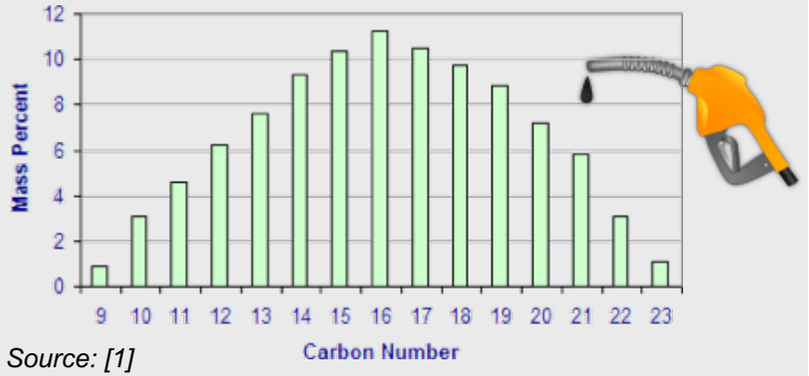
Source: [1]

Multicomponent fuel is the standard in diesel engine operation

[1] https://images.app.goo.gl/NSaXBLGtgLtTLs828

Motivation and Outline

Diesel fuel:



Source: [1]

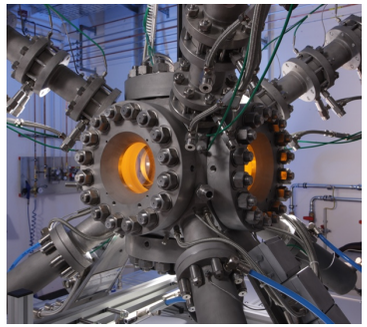
- Mixture of hundreds of hydrocarbons
- Exact composition neither known nor standardized
- Single species' interactions rather complex to investigate in such multicomponent mixtures

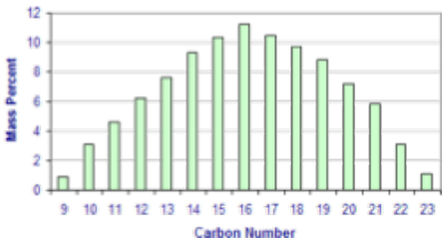
Aim:

- Investigation of multicomponent mixture influence along diesel engine cause and effect chain
- Based on simplified surrogate fuel:
  10 mass-% n-dodecane/
  90 mass-% n-heptane
- Based on application relevant configuration (spray chamber, near to application heavy-duty injector)

[1] https://images.app.goo.gl/NSaXBLGtgLtTLs828

Motivation and Outline



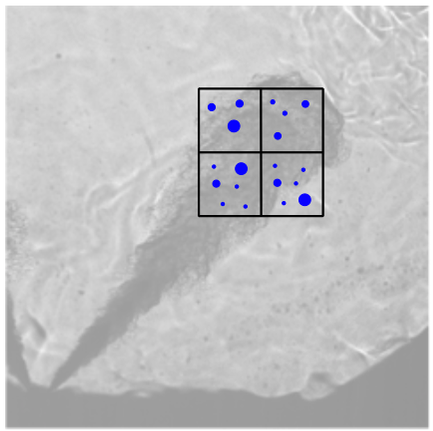


Source: [1]

Motivation

Experimental setup

Modeling Approach

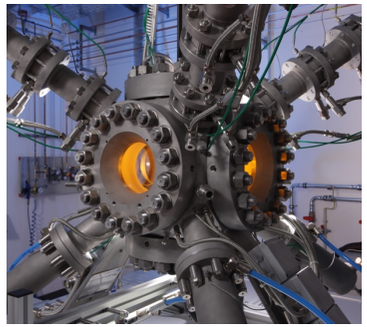


Results and Discussion

Summary and Outlook

[1] https://images.app.goo.gl/NSaXBLGtgLtTLs828

Motivation and Outline



Summary and Outlook

Results and Discussion

Modeling Approach

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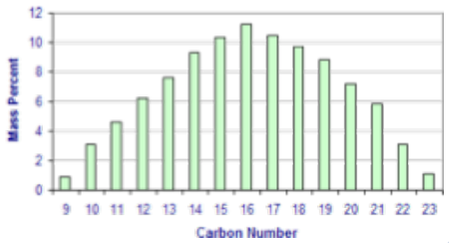

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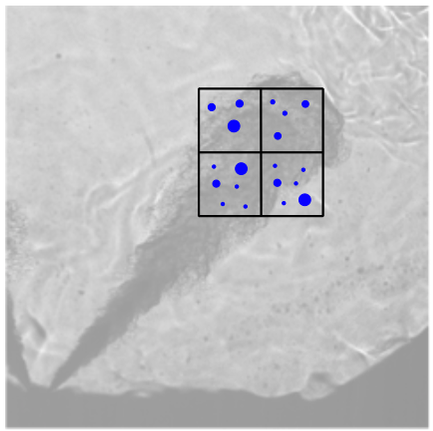

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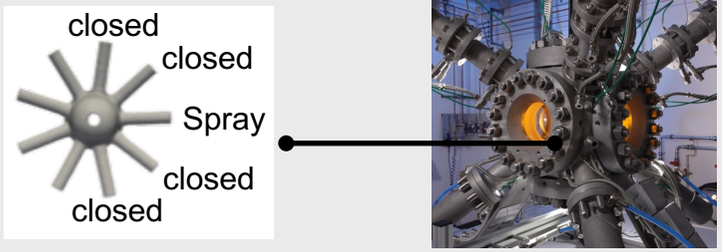
Experimental setup and techniques

Experimental setup:

- High pressure combustion chamber

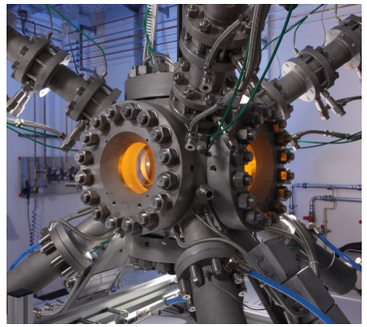


- Heavy-duty 9-hole injector, 4 holes closed
- Fuels
  - n-dodecane
  - n-dodecane / n-heptane mixture (10 / 90 mass-%)
- Chamber temperature: 600 °C
- Chamber pressure: 50 bar
- Rail pressure: 1000 bar
- Fuel temperature: 90°C

Experimental techniques:

- Inert environment (N_2):
  - μLIF (primary break-up)
  - Mie (liquid penetration)
  - Schlieren (vapor penetration)
- Reactive environment (air):
  - OH* luminosity
  - (Visual flame signal)

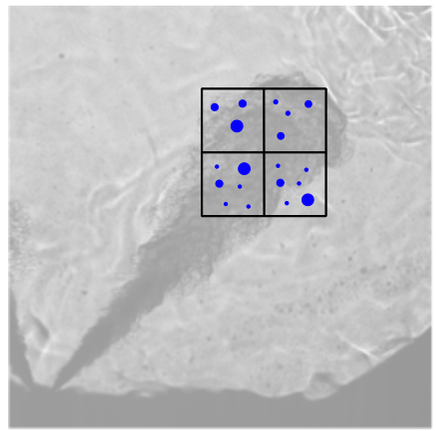
Motivation and Outline



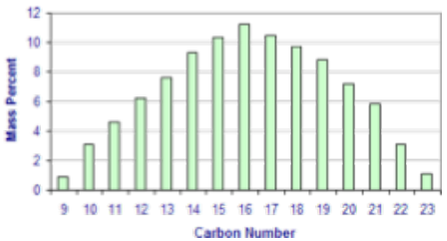
Summary and Outlook

Results and Discussion

Modeling Approach



Experimental setup



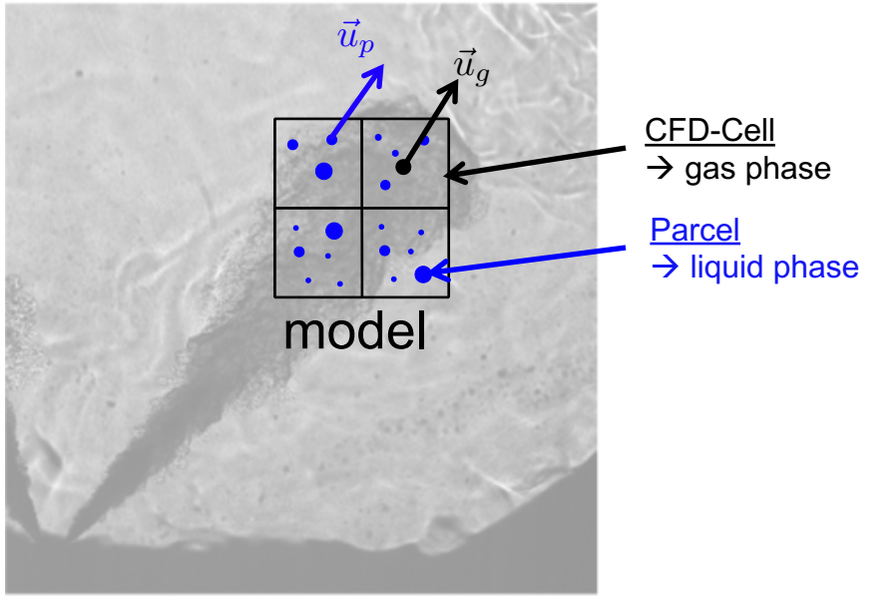
Source: [1]

Motivation

[1] https://images.app.goo.gl/NSaXBLGtgLtTLs828

Numerical approach for spray modeling

- Particle in cell method (PIC) / Euler – Lagrange Approach
  - Statistical description
  - Follows evolution of parcels
  - Each parcel represents collection of identical droplets



Source of Schlieren image: [1]

- Exemplary simulation result

Suitable approach for parcel (spray) initialization needed.

[1] L. Weiss, A. Peter, M. Wensing, „Diesel Spray characterization with Schlieren-Mie Technique“, Lisbon Symposia, Lisbon 2016

Inner nozzle flow and primary break-up

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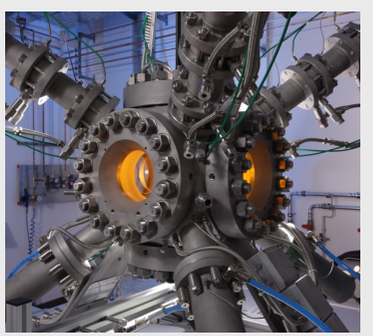
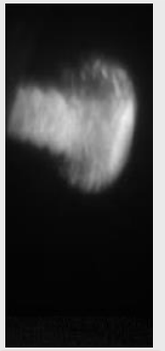
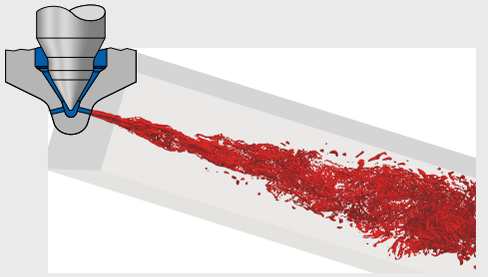
- μLIF data from high pressure injection chamber
  - T = 600 °C,
  - p = 50 bar
  - n-Dodecane





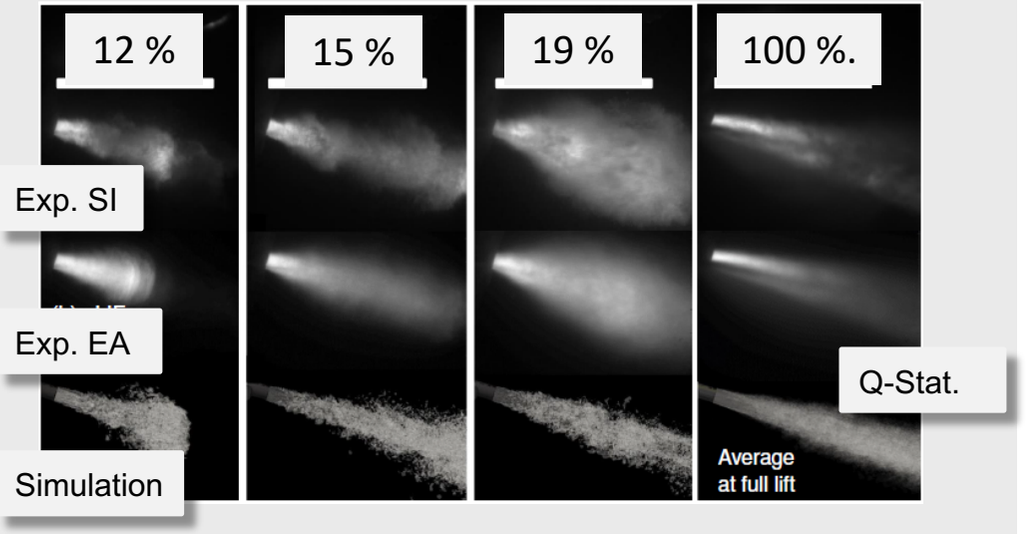
LTT ERLANGEN

- 3-Phase solver has been developed [1] and implemented in FoamExtend branch
- Liquid and vapor fuel, non-condensable gas
- 360° model of injector with directly coupled spray domain for one selected nozzle hole



HSM

- Opening phase
- Experimental μLIF data [2]
- Single shot (SI)
- Ensemble average (EA)
- Sim.: Iso-Surf. of liquid volume fraction



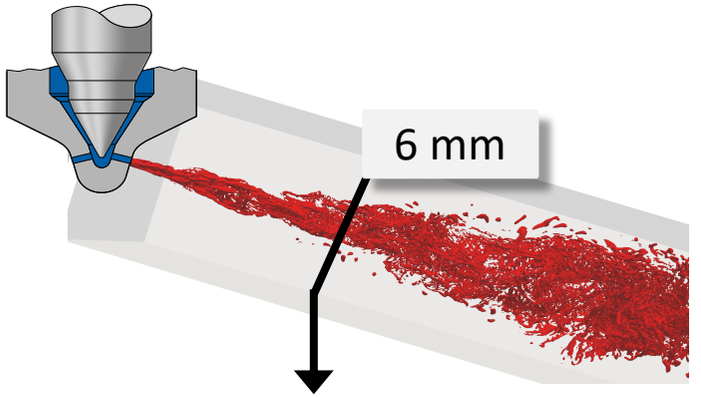
Agreement between simulation and experimental data in range of the cyclic fluctuations

[1]: Blume et al., submitted to Atomization&Sprays
[2]: L. Weiß, M. Wensing, FAU Erlangen-Nürnberg, 2018

In-nozzle flow / Spray interface

Lagrange spray initialization by PDF of ligament location, velocity and diameter

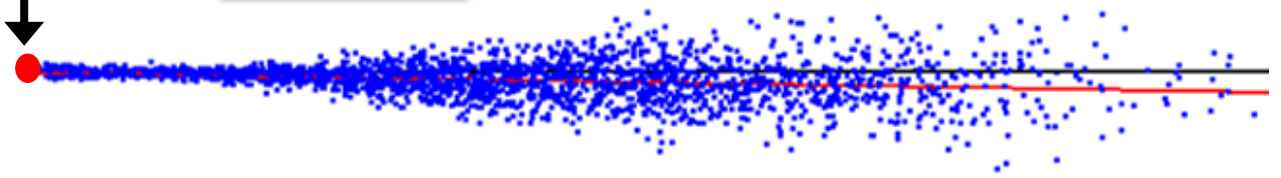
Euler VoF Simulation



$$f(d,u,r,\theta) \approx f(d) \cdot f(u|d) \cdot f(r|d) \cdot f(\theta|d,r)$$

Joint PDF

Coupled Euler-Lagrange Simulation



Spray asymmetry due to injector characteristics captured by simulation interface (joint PDF)

Evaporation model

- Particle in cell method (PIC) / Euler – **Lagrange** Approach
  - Liquid phase: Governing equation for each parcel in Lagrangian manner
  - Gas film transport equation (i... fuel and environment species):

$$\frac{d}{dr}\left(r^2\rho^g u Y_i^v - \rho_g \mathcal{D}_i^g r^2 \frac{dY_i^v}{dr}\right) = 0$$

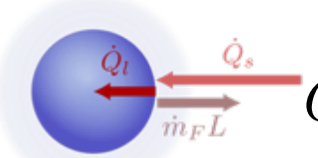
- Evaporation rate with convective fluxes:

$$\dot{m}_{f,i} = 2\pi r_d \frac{\lambda_g}{c_{p,g}} \mathrm{Nuln}\left(1 + B_{m,i}\right)$$

$$B_{m,i} = \frac{Y_{f,i}^s - Y_{f,i}^\infty}{1 - Y_{f,i}^s}$$

$$\mathrm{Nu} = 2 + 0{,}6\mathrm{Re}^{1/2}\mathrm{Pr}^{1/3}$$

- Droplet temperature

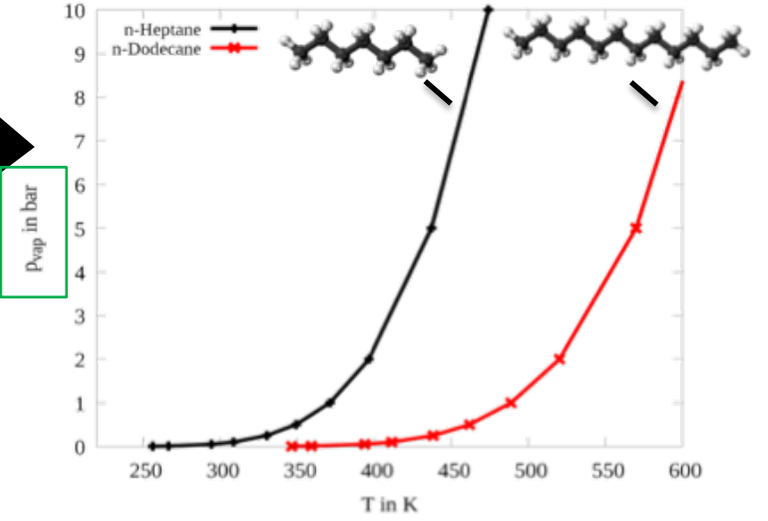


$$\dot{Q}_l = \dot{Q}_s - \dot{m}_F L$$

$$\frac{dT_d}{dt} = \frac{\dot{Q}_s - \dot{m}_F L}{m_d c_{p,l}}$$

- Raoult's law for vapor-liquid equilibrium at interface:

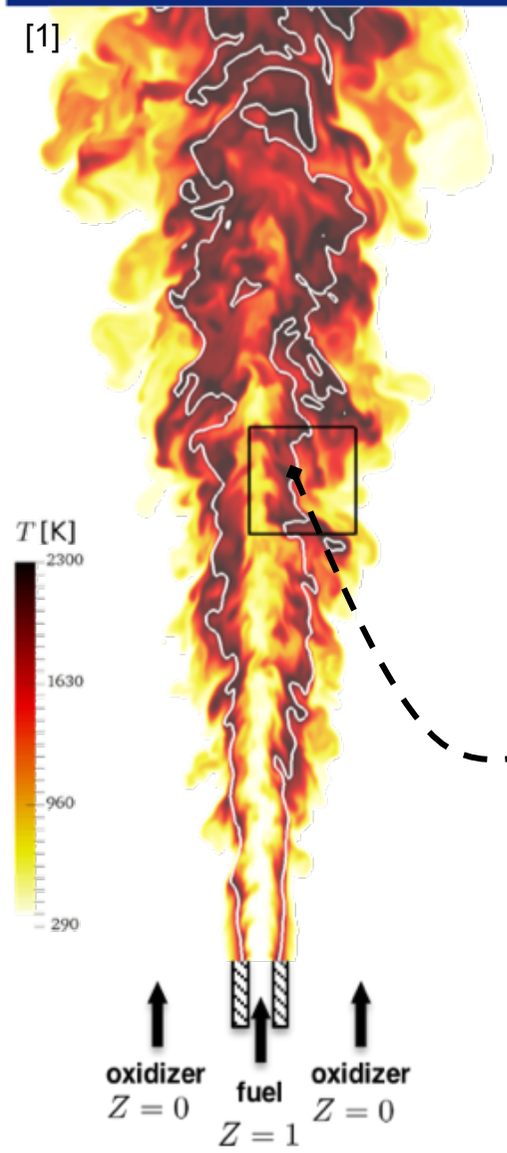
$$X_{f,i}^s = X_{f,i}^l \frac{p_{vap,i}}{p}$$



n-heptane evaporating faster than n-dodecane

Combustion model – Flamelet concept

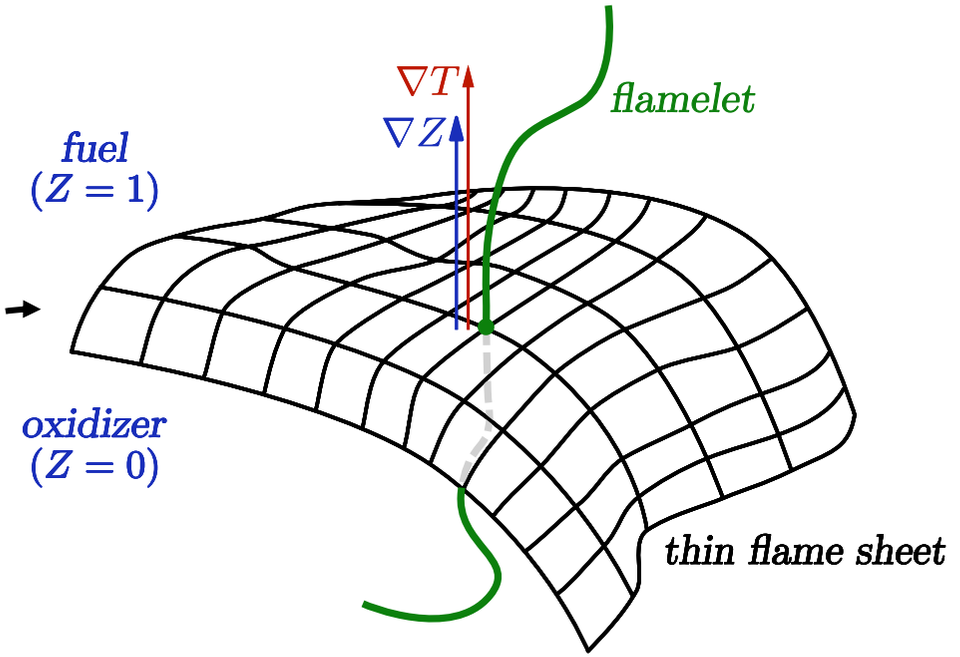
[1]



Theoretical basis of the flamelet concept:

- combustion chemistry is fast
- **thin flame sheet** assumption
- **gradient alignment** at flame sheet
- important physics along **flame-normal** direction

Definition: $Z = \dfrac{m_{\text{fuel}}}{m_{\text{fuel}} + m_{\text{oxid}}}$



$$\rho \frac{\partial Y_i}{\partial \tau} = \frac{\rho \chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i$$

$$\rho \frac{\partial T}{\partial \tau} = \frac{\rho \chi}{2} \frac{\partial^2 T}{\partial Z^2} + \dot{\omega}_T$$

$$\chi = 2D|\nabla Z|^2$$

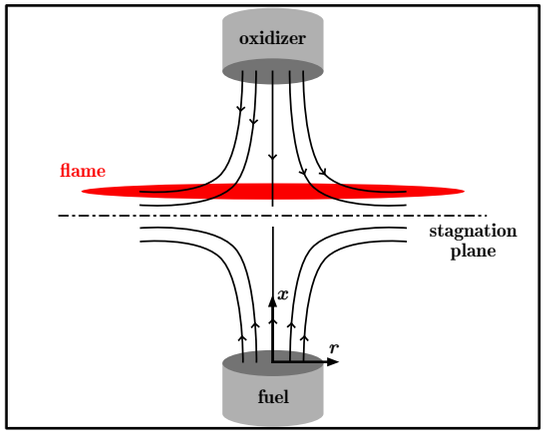
[2]

Turbulent flames ≈ Ensembles of 1D flamelets

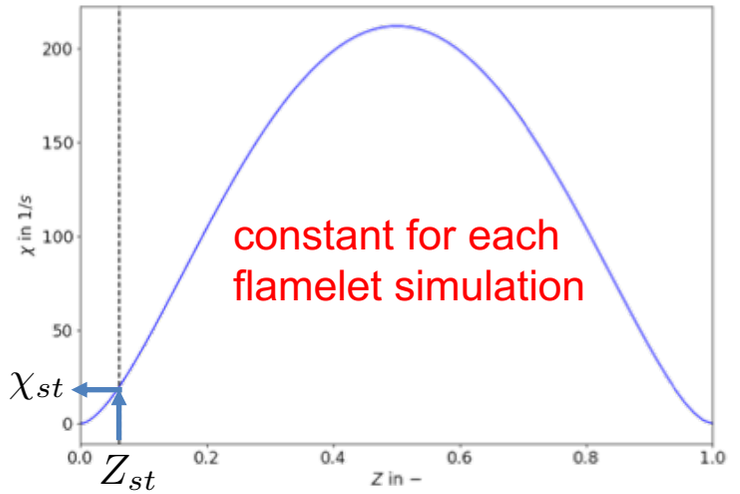
[1] Popp, STFS, 2015
[2] N. Peters. Symp. (Int.) Combust. 21 (1988)

Combustion model – Flamelet concept spray

- $\chi(Z)$ obtained from canonical setups, e.g. counterflow diffusion flame



$$\chi(Z) = \chi_{st}\exp(2[\mathrm{erfc}^{-1}(2Z_{st})]^2 - 2[\mathrm{erfc}^{-1}(2Z)]^2)$$



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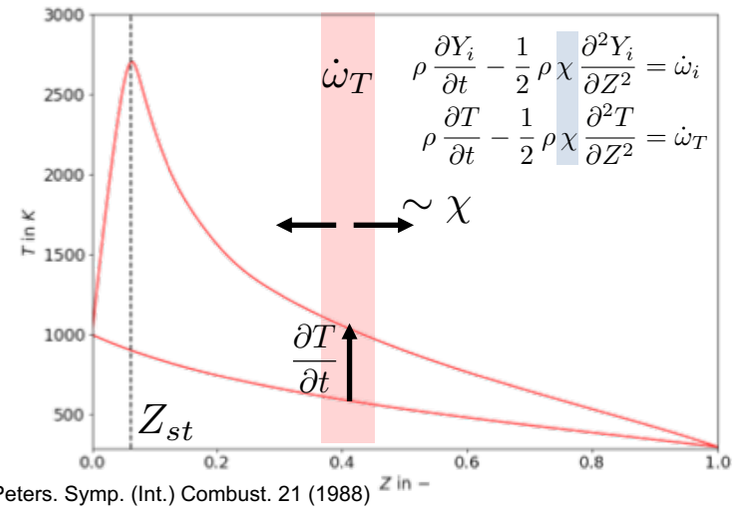
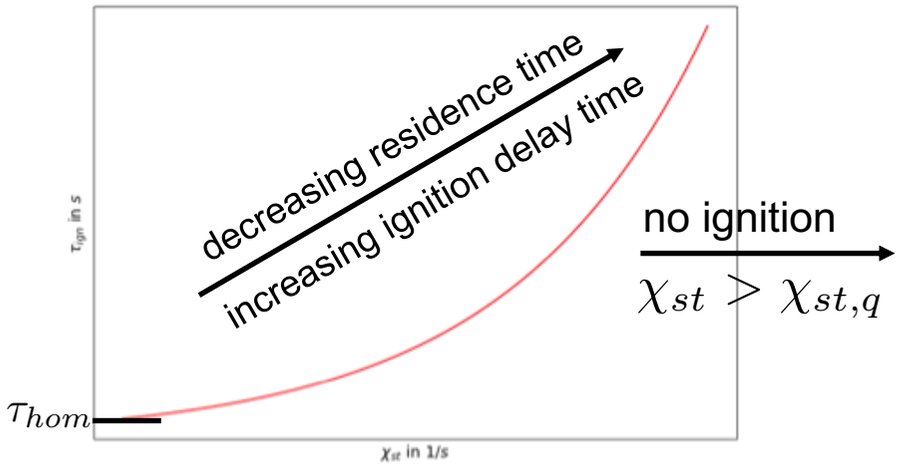
[1]

- As diffusion coefficient, χ acts as inverse residence time for fluid packages in mixture fraction space → determines ignition delay time

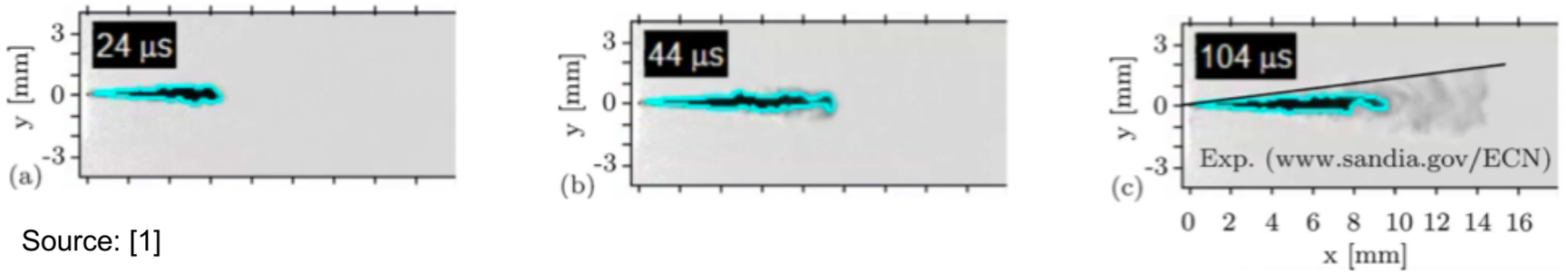




[1 N. Peters. Symp. (Int.) Combust. 21 (1988)

Combustion model – Flamelet concept spray

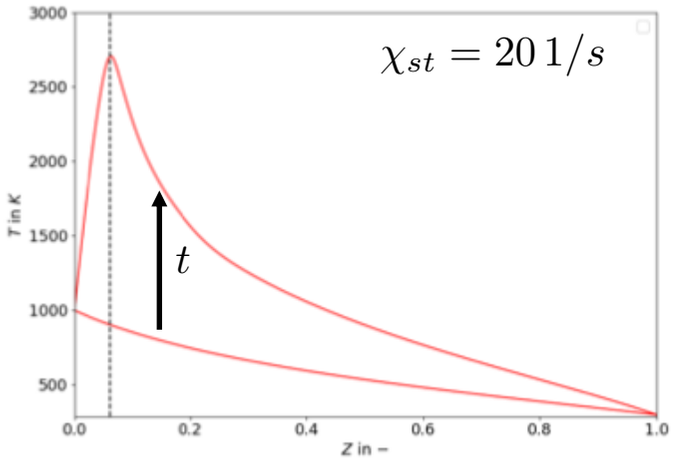
- In diesel sprays, χ_{st} is varying after start of injection and not known a-priori (function of nozzle and injection parameters)



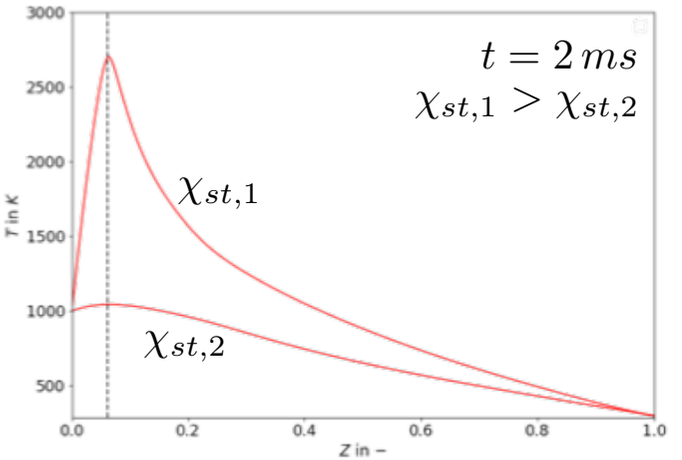
Source: [1]

- Tabulation of flame structures based on constant χ_{st} simulations chosen here to capture main effects of the combined ignition and mixing processes with manageable effort

Progress of ignition → Progress variable Y_C



Impact of scalar dissipation rate χ_{st}



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$$\chi = 2D|\nabla Z|^2$$

[1]

[1]: Pickett, L. M., Genzale, C. L., Manin, J., Malbec, L. M. & Hermant, L. 2011 Measurement uncertainty of liquid penetration in evaporating Diesel sprays. In Proceedings of the 23rd Annual Conference on Liquid Atomization and Spray Systems

Combustion model – Flamelet concept bi-component spray

- Parametrization of fuel composition for 2 components:

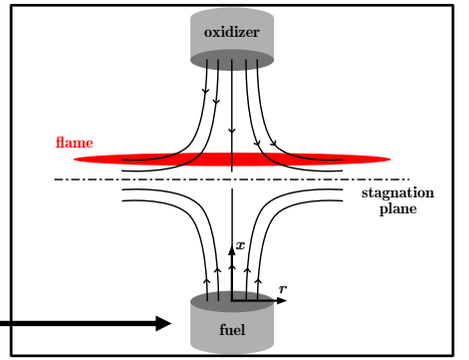
$$Z_{\mathrm{C12H26}} = \frac{m_{\mathrm{g,ox,Cl2H26}}}{m_g + m_{\mathrm{g,Cl2H26}} + m_{\mathrm{g,C7H16}}} = Z_1$$

$$Z_{\mathrm{C7H16}} = \frac{m_{\mathrm{g,C7H16}}}{m_g + m_{\mathrm{g,Cl2H26}} + m_{\mathrm{g,C7H16}}} = Z_2$$

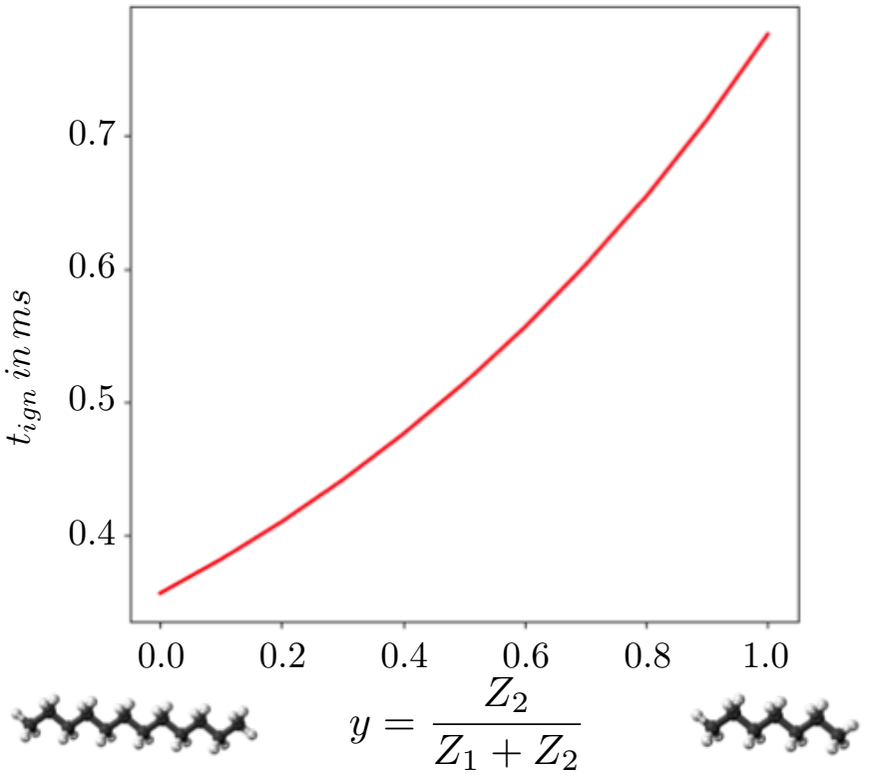
- In more appropriate formulation:

$Z = Z_1 + Z_2$ Location in Z-space

$y = \frac{Z_2}{Z_1 + Z_2}$ Composition of fuel

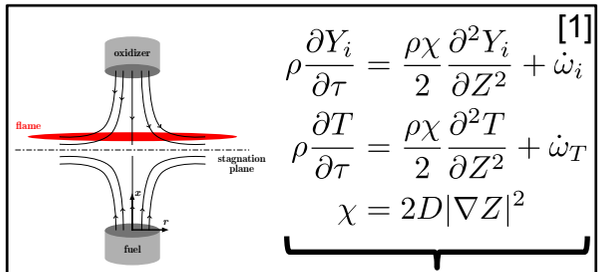


- Ignition delay obtained by flamelet simulation



Ignition delay time increasing with n-heptane content

Combustion model – Resulting tabulation approach



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$$\chi = 2D|\nabla Z|^2$$

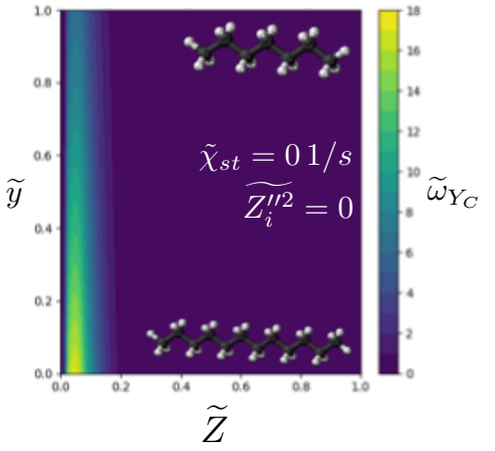
[1]

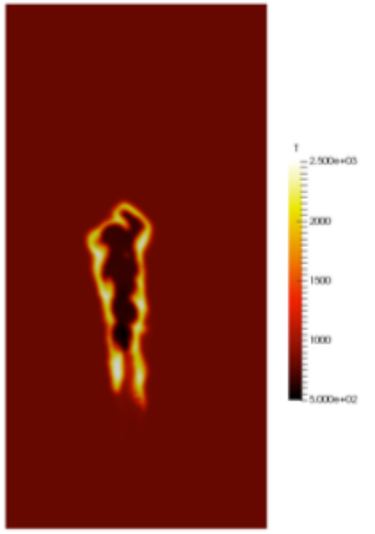
Thermo-chemical state

$$Z = Z_1 + Z_2$$

$$y = \frac{Z_2}{Z_1 + Z_2}$$

Fuel composition





tabulation
+ 2D β-pdf integration

coupling

1D Flamelet

Full Thermochemical State
$\Psi = [T, Y_1, Y_2, ..., Y_{n_s}]$

Database

Reduced-order Model
$\tilde{\Psi} = \tilde{\Psi}\left(\tilde{y}, \tilde{Z}, \widetilde{Z''^2}_{sum,n}, \tilde{\chi}_{st}, \tilde{Y}_C^{\text{norm}}\right)$

CFD

Solve control variables
$\tilde{Z}_1, \tilde{Z}_2, \tilde{Y}_C$ instead of $\tilde{\Psi}$

[1] N. Peters. Symp. (Int.) Combust. 21 (1988)

Combustion model – Chemical mechanism

- Tabulated chemistry enables incorporation of complex chemical mechanism in 3D-CFD
- But: Amount of flamelet simulations makes utilization of reduced mechanism advantageous
- Reduction approach:

Preselection based on heaviest fuel components

Reduction procedure utilizing DRGEP + SA [1,2,3]

POLIMI C0-C16 mechanism (Low/High Temperature)
- ~ 500 species
- ~ 17000 reactions


Source: [4]

POLIMI TPRF mechanism (Low/High Temperature)
- ~ 335 species
- ~ 9315 reactions

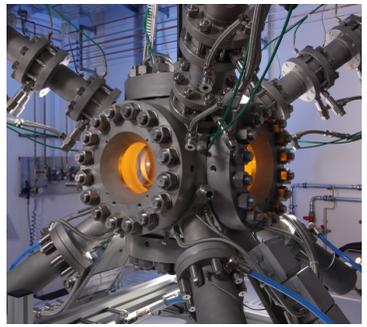
Reduction (DRGEP + SA)

C12-C7 reduced mechanism (Low/High Temperature)
- ~ 127 species
- ~ 2205 reactions

- Optimization target: Homogeneous ignition delay time
- A-posteriori evaluation based on laminar flame speed and diffusion flames relevant for current spray flame tabulation

[1]: Pepiot-Desjardins, P., & Pitsch, H. (2008). An efficient error-propagation-based reduction method for large chemical kinetic mechanisms. Combustion and Flame, 154(1-2), 67-81.,
[2]: Niemeyer, K. E., Sung, C. J., & Raju, M. P. (2010). Skeletal mechanism generation for surrogate fuels using directed relation graph with error propagation and sensitivity analysis. *Combustion and flame*, *157*(9), 1760-1770.
[3]: Stagni, A., Frassoldati, A., Cuoci, A., Faravelli, T., & Ranzi, E. (2016). Skeletal mechanism reduction through species-targeted sensitivity analysis. Combustion and Flame, 163, 382-393.
[4]: http://creckmodeling.chem.polimi.it/menu-kinetics

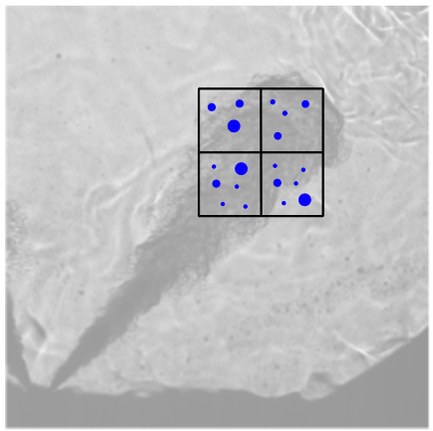
Motivation and Outline



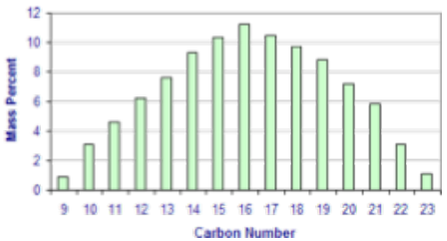
Summary and Outlook

Results and Discussion

Modeling Approach



Experimental setup



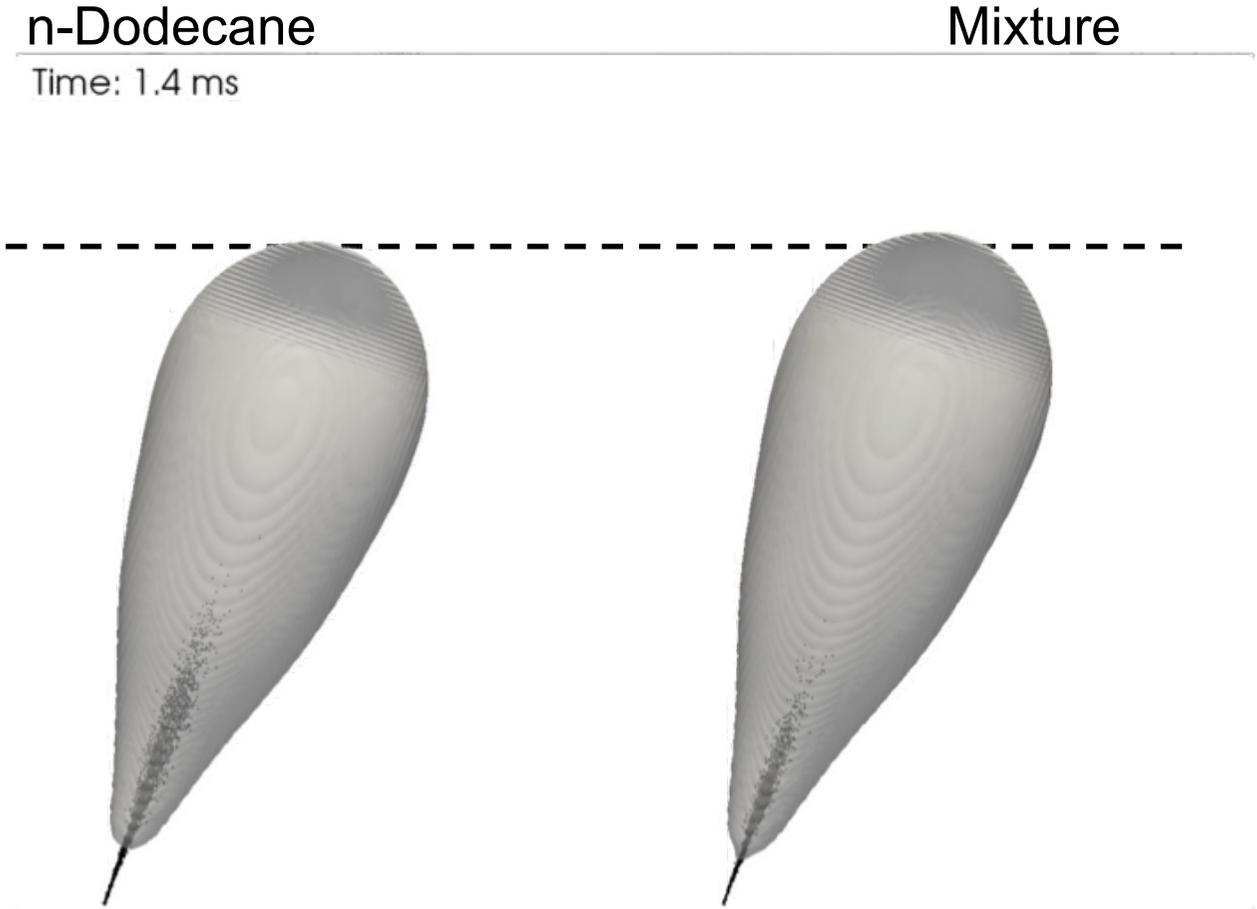
Source: [1]

Motivation

[1] https://images.app.goo.gl/NSaXBLGtgLtTLs828

Investigation mixing field in non-reactive environment

- Comparison of evaporation behavior and mixture formation based on 1% fuel mass fraction:



- Initial fuel vapor earlier for mixture than for pure n-dodecane
- Vapor penetrations similar for both fuels

Differences in start of fuel vapor formation with similar vapor penetration length

Comparison vapor and liquid penetration in non-reacting environment

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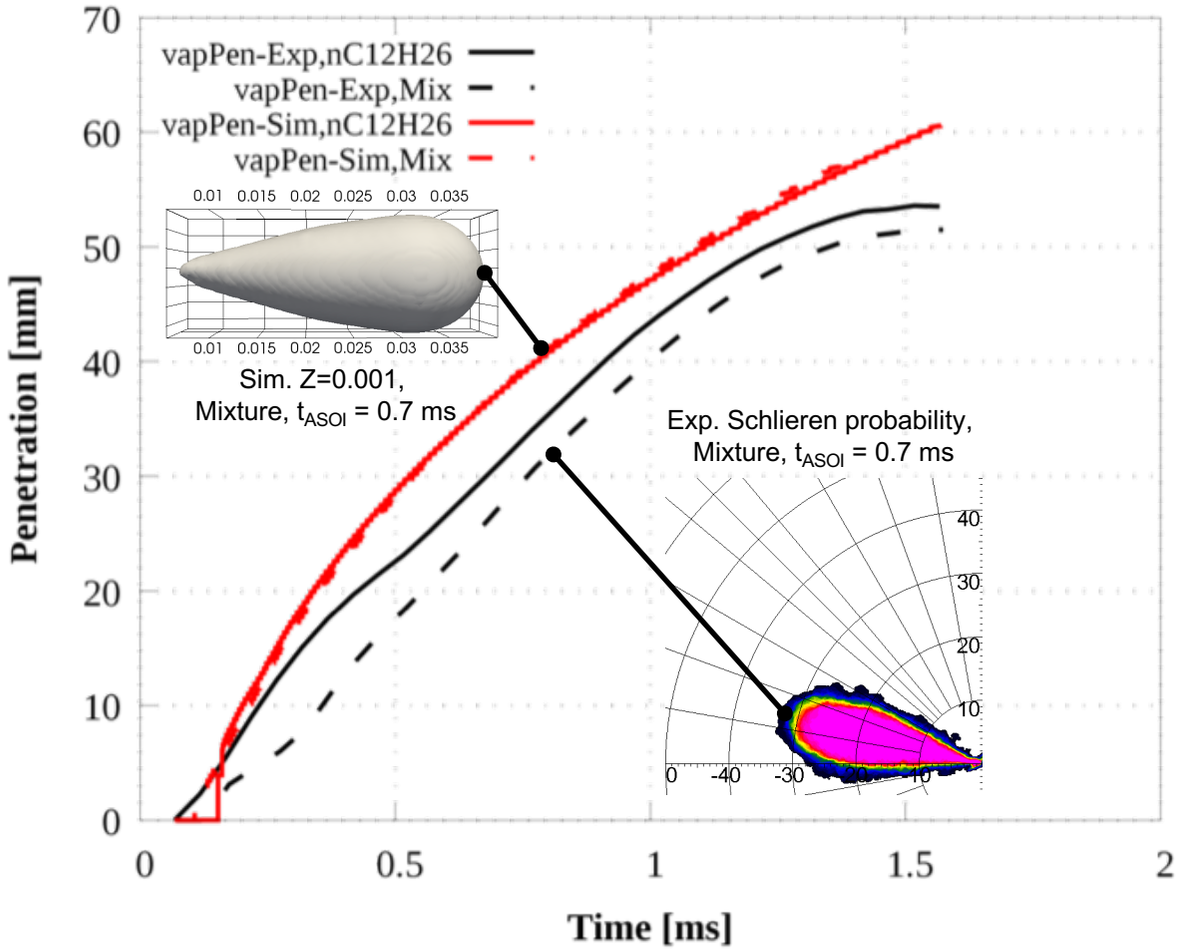
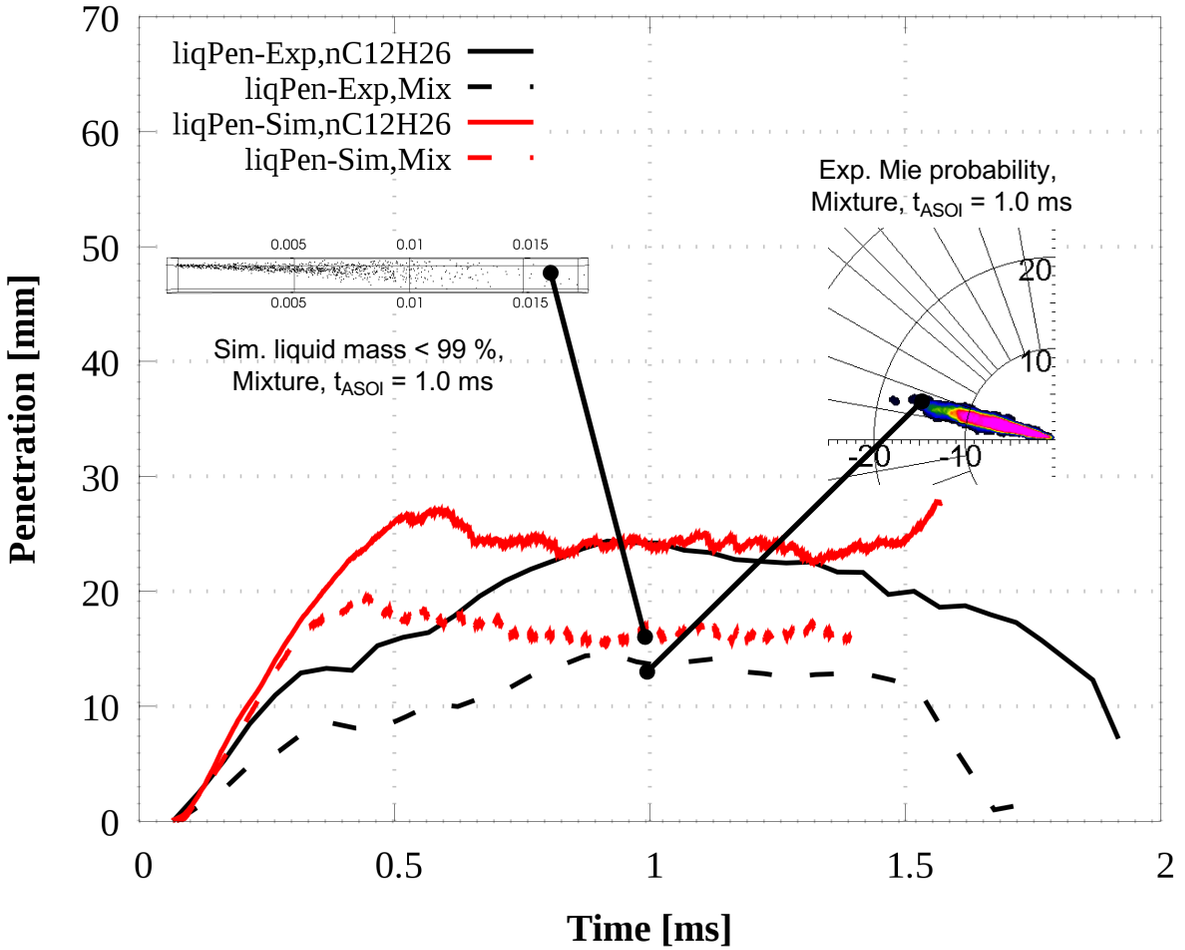
- Validation of vapor and liquid penetration lengths



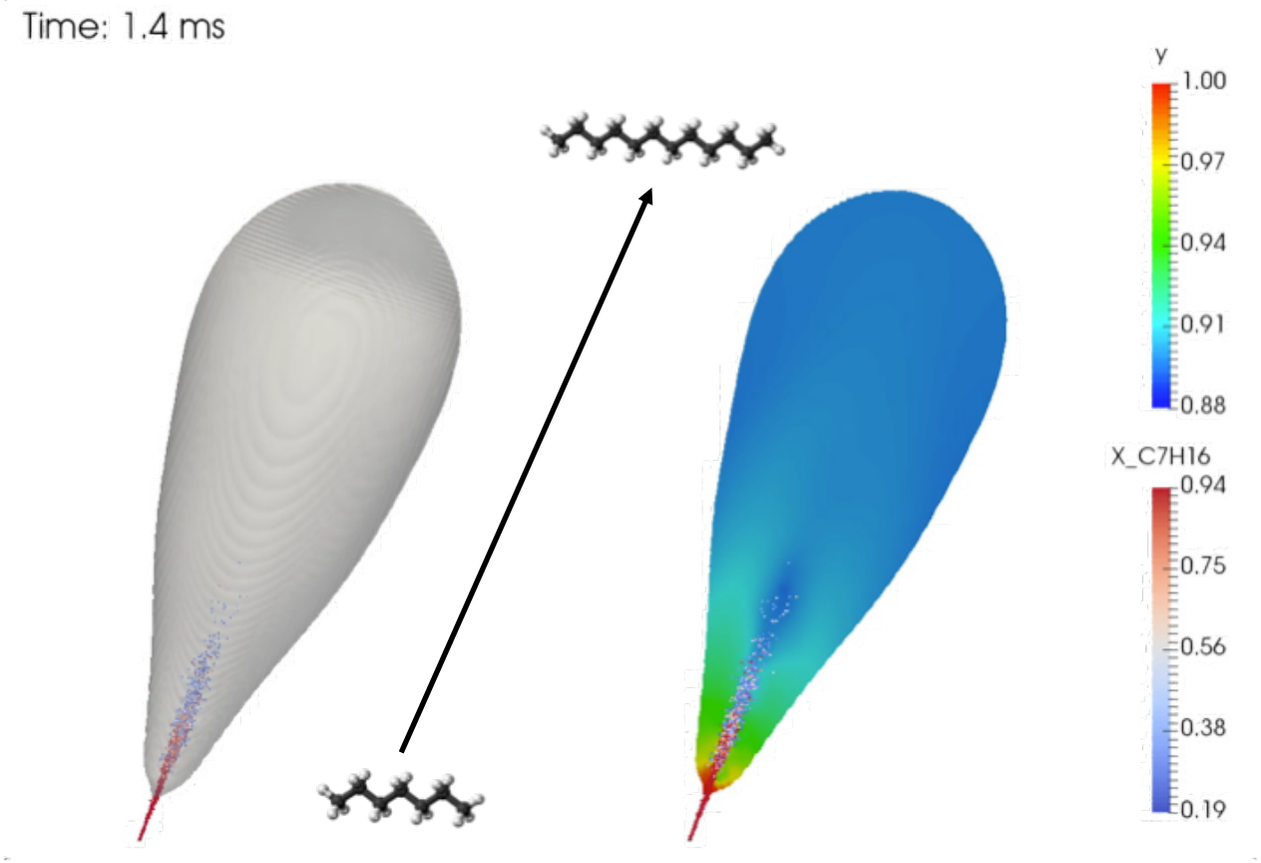
Vapor penetration slightly overpredicted, no fuel influence in simulation



Steady liquid penetration in agreement with exp. data, fuel influence captured

Investigation gaseous fuel composition in non-reactive environment

- Comparison of liquid and gas phase composition:



- Downstream reduction of n-heptane fraction in
  - Liquid phase
  - Gas phase

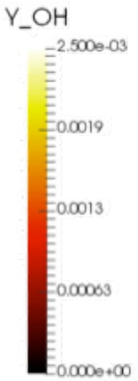
High fraction of n-heptane in liquid and vaporized fuel, decreasing with distance to injector

Comparison ignition and combustion process

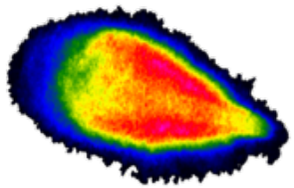
- Simulation results for ignition and combustion behavior

n-Dodecane

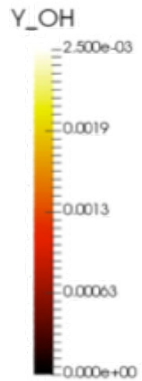
Time: 0.7 ms



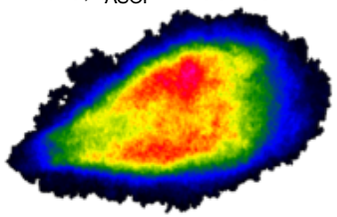
Exp. line of side integrated OH*
n-Dodecane, t_{ASOI} = 0.70 ms



Mixture



Exp. line of side integrated OH*
Mixture, t_{ASOI} = 1.05 ms

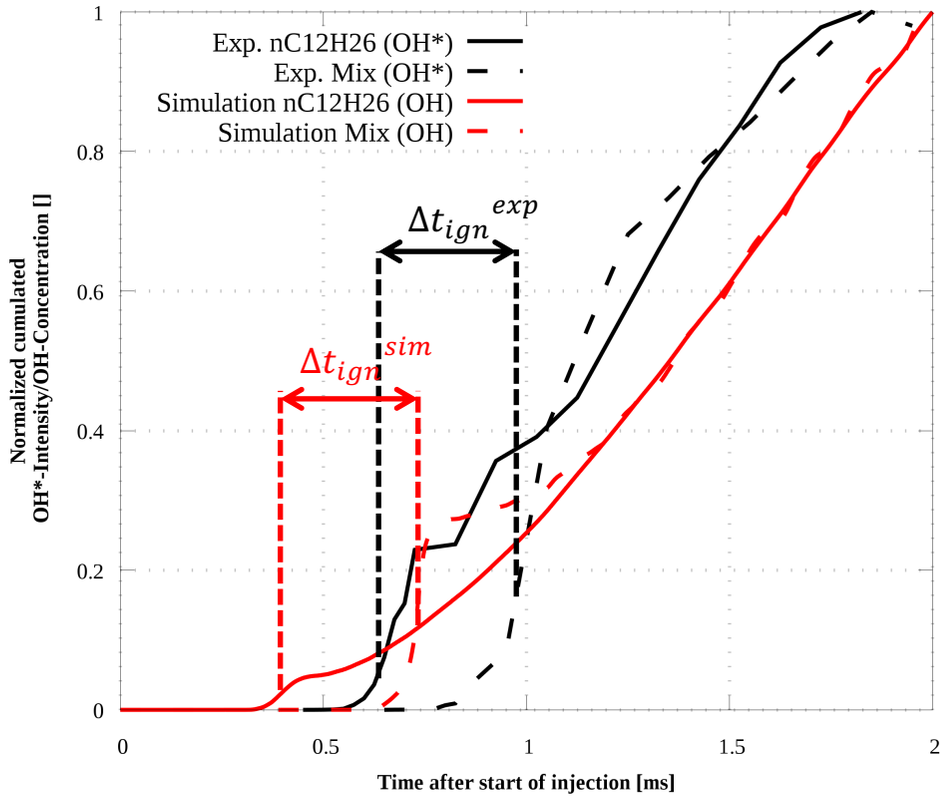


- Combustion starts at spray flank and proceeds towards spray tip
- Ignition delay time smaller for pure n-dodecane than for mixture

Qualitative experimental findings concerning ignition process reproduced, n-heptane content in gas phase increases ignition delay time

Comparison integrated OH* and OH signal

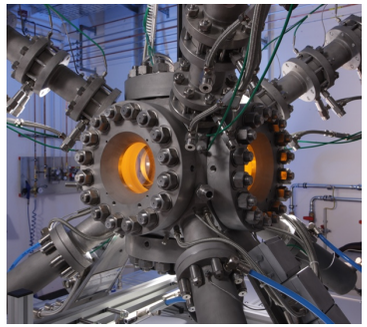
- Comparison of ignition delay times based on cumulated OH* signal (exp.) / OH mass fraction (sim.)

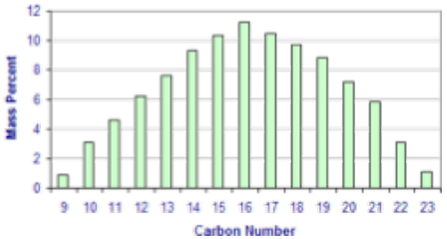


- Ignition delay time slightly underpredicted by simulation for both, pure n-dodecane and mixture
- But: Difference in ignition delay time of n-dodecane and mixture well reproduced

Differences in ignition delay time captured by tabulation strategy

Motivation and Outline





Source: [1]

Motivation

Experimental setup

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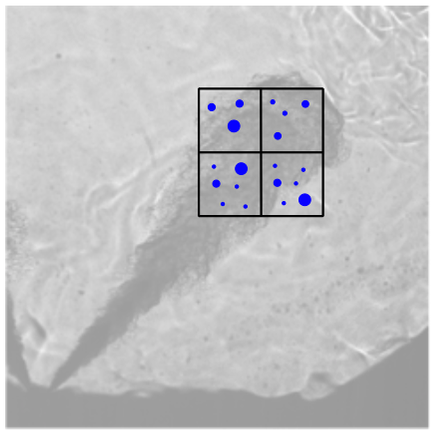


Results and Discussion

Summary and Outlook

[1] https://images.app.goo.gl/NSaXBLGtgLtTLs828

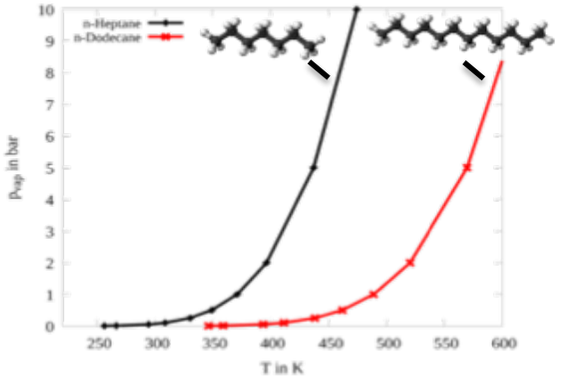
Summary and Outlook

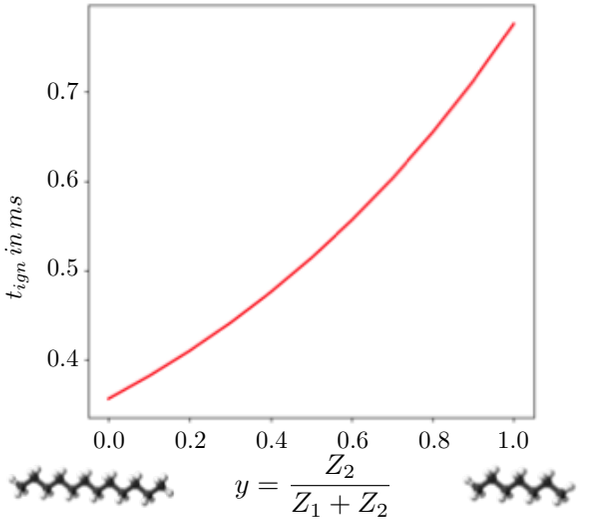
Aim:

- Investigation of multicomponent mixture influence along diesel engine cause and effect chain
- Based on simplified surrogate mixture:
  10 mass-% n-dodecane/
  90 mass-% n-heptane
- Based on application relevant configuration (spray chamber, near to application heavy-duty injector)

Findings:

- Liquid penetration for mixture shorter than for pure n-dodecane
- Initial fuel vapor first formed by mixture
- Simulated vapor penetration unaffected by fuel composition due to same injection pressure / similar momentum flux
- Ignition delay time for surrogate larger than for n-dodecane due to n-heptane content in gas phase





Outlook:

- LES of setup to investigate influence of gas phase mixing model

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- with computing resources granted by RWTH Aachen University within the computing project *bund0002*.

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Bundesministerium für Wirtschaft und Energie

aufgrund eines Beschlusses des Deutschen Bundestages

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