Combustion and Emission Modeling in CONVERGE with LOGE models

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LOGE
LUND COMBUSTION ENGINEERING

Outline

- Objective
- LOGE models for Diesel Engine Modeling
  - Combustion: LOGE TIF – Transient Interactive Flamelet
  - Soot emissions: LOGE FSM – Fixed Shape Moments
- Coupling with CONVERGE
- Diesel Engine Application
- Summary and Conclusion

Objective

- Improved prediction of
  - Combustion
  - Soot emissions
  - Soot/NOx –tradeoff

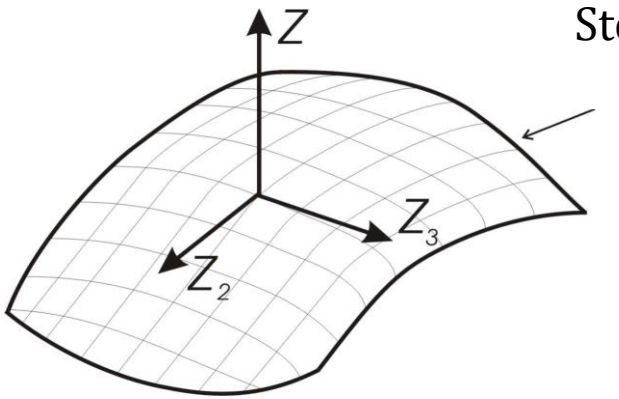
  … for part load, high EGR Diesel engine operating points

- Modeling of multiple injections with the Transient Interactive Flamelet model
- Combustion modeling with a dedicated Diesel fuel surrogate chemical mechanism
- Improved soot prediction using "Fixed Shape Moments"

COMBUSTION MODELING

LOGE TIF

LOGEsoft TIF



Stoichiometric mixture isosurface

Main feature:
Allows decoupling of flow and chemistry
Mixture fraction *Z*:
"Mass originating from fuel stream"
Scalar dissipation rate χ:
"Diffusion rate in mixture fraction space"

Scalar transport equation :

$$\rho \frac{\partial Y_i}{\partial t} + \rho v_\alpha \frac{\partial Y_i}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha}\left(\rho D \frac{\partial Y_i}{\partial x_\alpha}\right) = \dot{\omega}_i$$

Scalar dissipation rate

$$\chi \equiv 2D\left(\frac{\partial Z}{\partial x_\alpha}\right)^2$$

Flamelet transform:

$$\begin{cases} \dfrac{\partial Y_i}{\partial t} = \dfrac{\partial Y_i}{\partial \tau} + \dfrac{\partial Z}{\partial t}\dfrac{\partial Y_i}{\partial Z} \\ \dfrac{\partial Y_i}{\partial x_1} = \dfrac{\partial Z}{\partial x_1}\dfrac{\partial Y_i}{\partial Z} \\ \dfrac{\partial Y_i}{\partial x_\alpha} = \dfrac{\partial Y_i}{\partial Z_\alpha} + \dfrac{\partial Z}{\partial x_\alpha}\dfrac{\partial Y_i}{\partial Z}, \alpha = 2{,}3 \end{cases}$$

Peters 1984

Equation in flamelet space

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

$$\tilde{\chi} = c_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \widetilde{Z''^2}$$

$$\tilde{Y}_i(x_\alpha) = \int Y_i(Z)\, \tilde{P}(x_\alpha; \tilde{Z}, \widetilde{Z''^2})\mathrm{d}Z$$

LOGE
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LOGEsoft TIF – Coupling with CONVERGE

- Multiple flamelets with flamelet-flamelet interaction model
- Coupling performed through UDF
  - User_combust_model
  - User_source_drivers_passive
  - User_post
- Parallelization:
  - Open-MPI compiled with Intel Fortran 95/2003 bindings
  - HP-MPI distributed with CONVERGE
- Uses the same parallel process environment as CONVERGE

Diesel Fuel Chemistry and Physical Properties

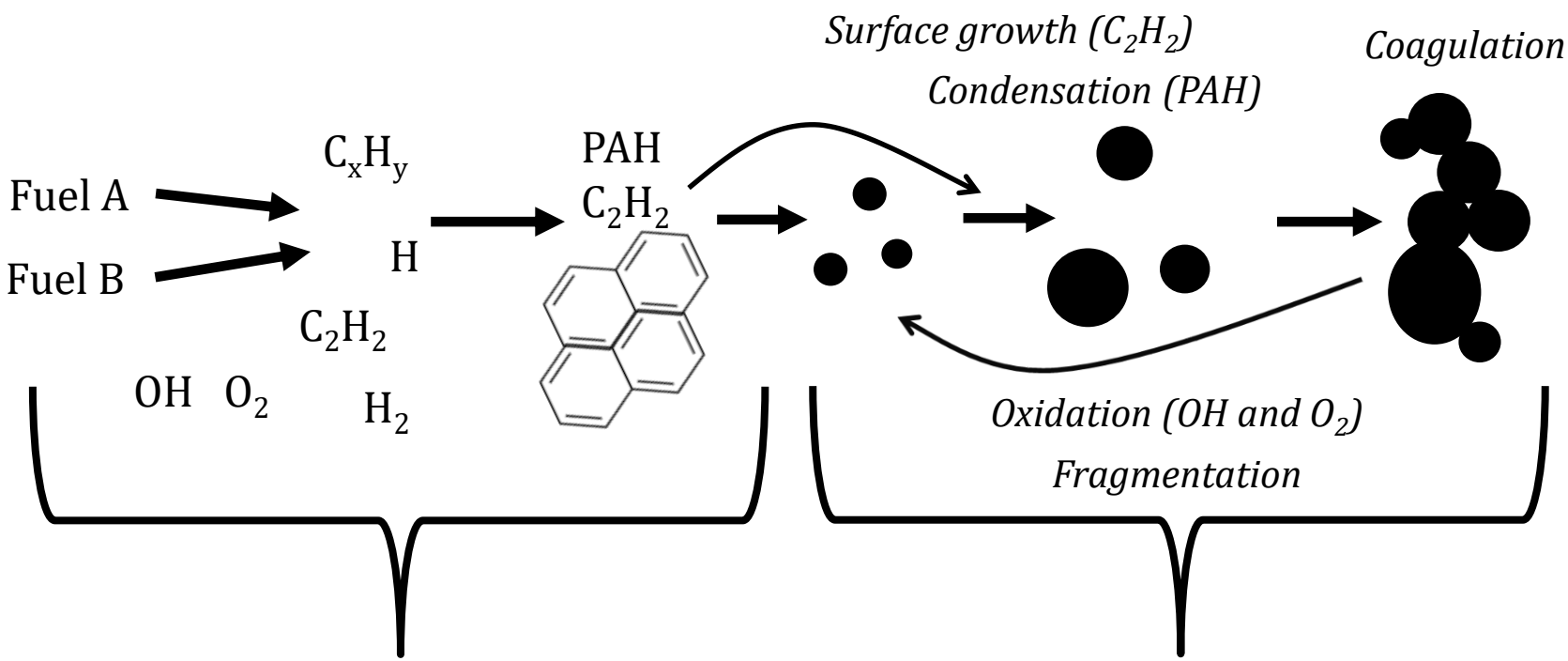
- Reaction mechanism
  - Latest LOGE DIESEL skeletal reaction scheme
    - 188 species (including PAH chemistry and NOx chemistry)
    - 1333 reactions
  - Composition determined according to fuel analysis
    - Amount of mono- and polyaromatics
    - C:H ratio and Lower Heating Value

Species	**Mass fraction**
Toluene	0.125
1-Methylnaphthalene	0.044
n-Decane	0.831

- LOGE DIESEL Liquid property database

SOOT MODELING
FIXED SHAPE MOMENTS

Soot modelling

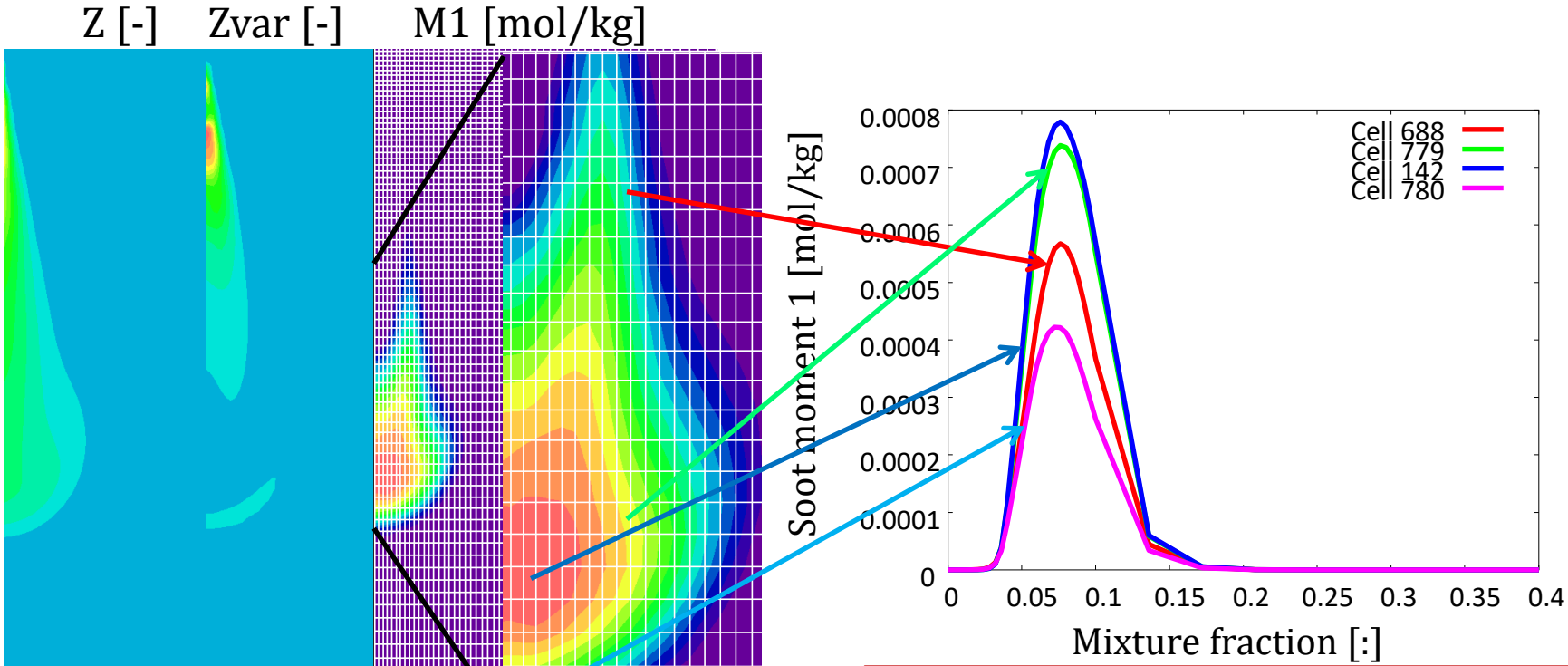


Gas-phase kinetics:
- Validation (laminar flames)
- Description of PAH formation
- Consistency

Soot Particle Size Distribution:
- Method of moments (PM)
- Sectional method (PSM)

Soot model: FSM (Fixed Shape Moments)

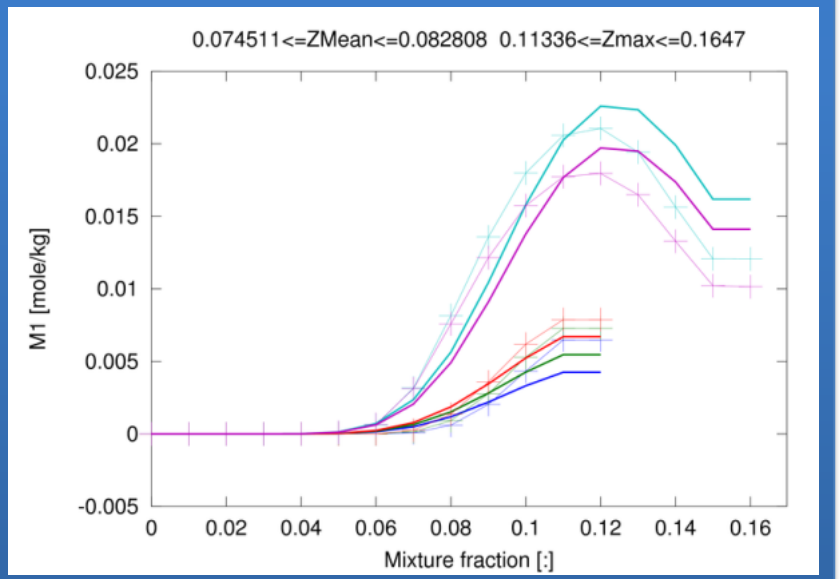
- A Conditional Moment Closure Calculation shows that it is important to consider the shapes of the soot moments in mixture fraction space
- In the FSM model, we use a parameterization of the soot moments in mixture fraction space to be able to consider sub-grid-scale effects



The soot moments are not constant in mixture fraction space

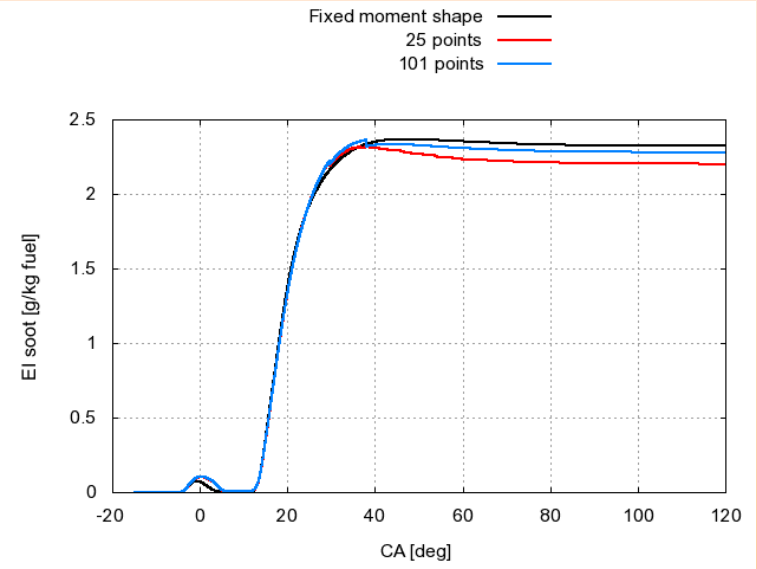
FSM: Mixture fraction space resolved soot moments

Soot $M_1(Z)$ for select cells



Comparison between parameterized (FSM solid lines) and resolved (CMC - +) soot moments at CA 20

Engine calculation - accuracy



High EGR part load OP

- CMC with 101 vs. 25 points
- Shape function (FSM)

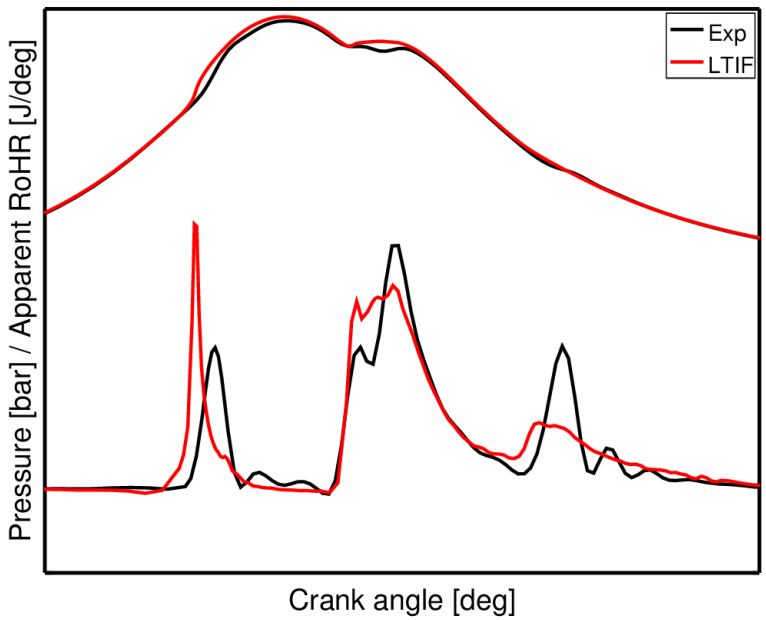
- The sub-grid-scale shape is parametrized as function of mixture fraction
- A very close match is acheived compared with soot CMC
- **FSM caters for cell local effects**
- **Soot source terms are taken from a flamelet library**

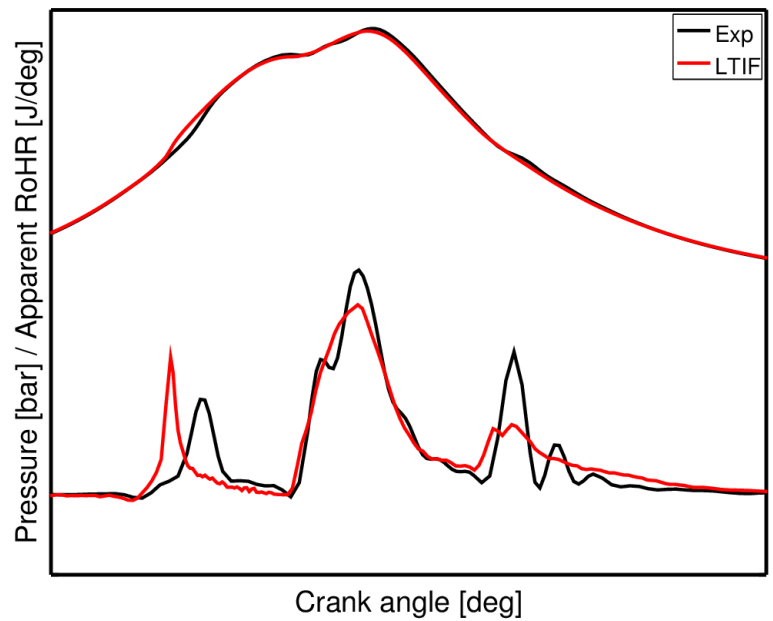
Summary – Combustion and Soot Modeling

	LOGE TIF	Fixed Shape Moments
Chemistry treatment	Online calculation	Flamelet table
Cell local resolution	No	Yes
Turbulence-chemistry interaction	Yes	Yes
Transport	Flamelet markers	Mean M_0 and M_1
Scalar dissipation rate treatment	Global	Cell local
PDF treatment	$\tilde{Z}$ and $\widetilde{Z''^2}$ in the cell	$\tilde{Z}$ and $\widetilde{Z''^2}$ in the cell
NOx, CO, UHC	PDF integrated from the interactive flamelets	
Soot		Cell local with sub-grid-shape function

DIESEL ENGINE APPLICATION

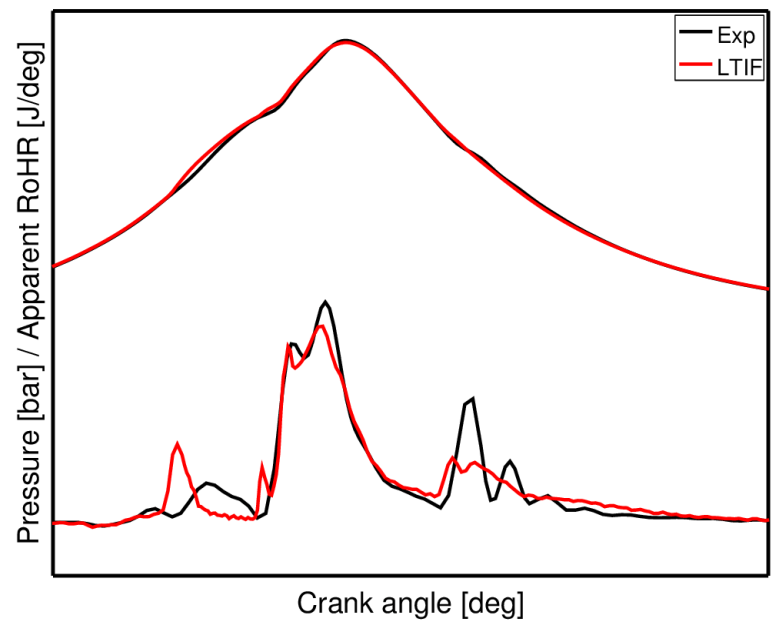
LTIF combustion prediction



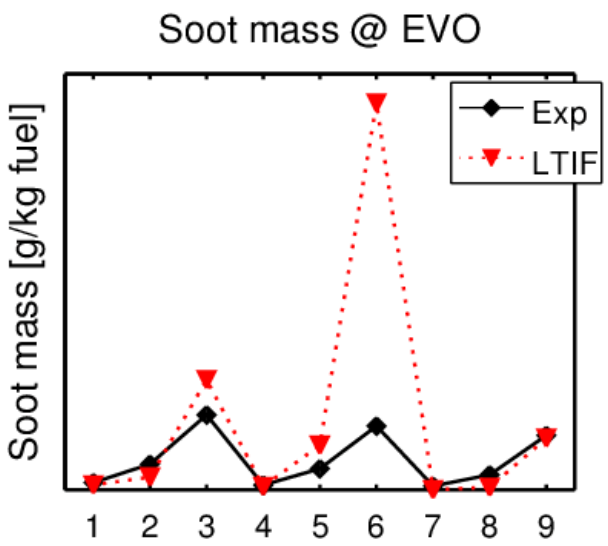


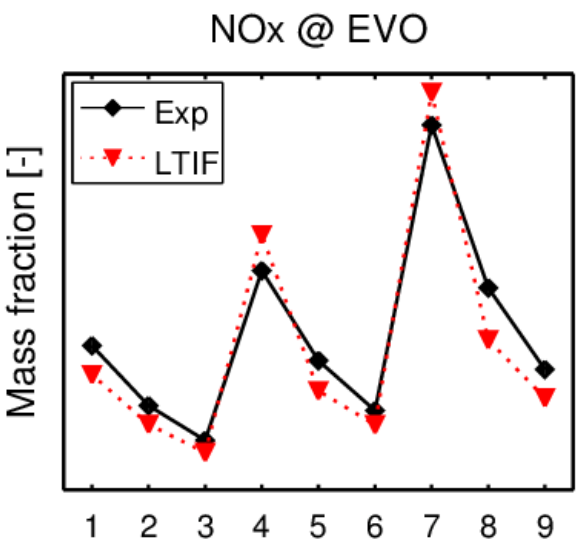
- 9 Cases:

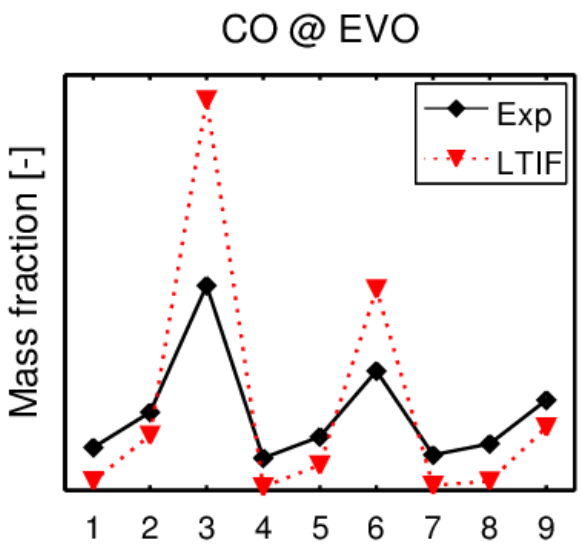
	EGR level 1	EGR level 2	EGR level 3
SOI 1	×	×	×
SOI 2	×	×	×
SOI 3	×	×	×



LTIF emissions all cases



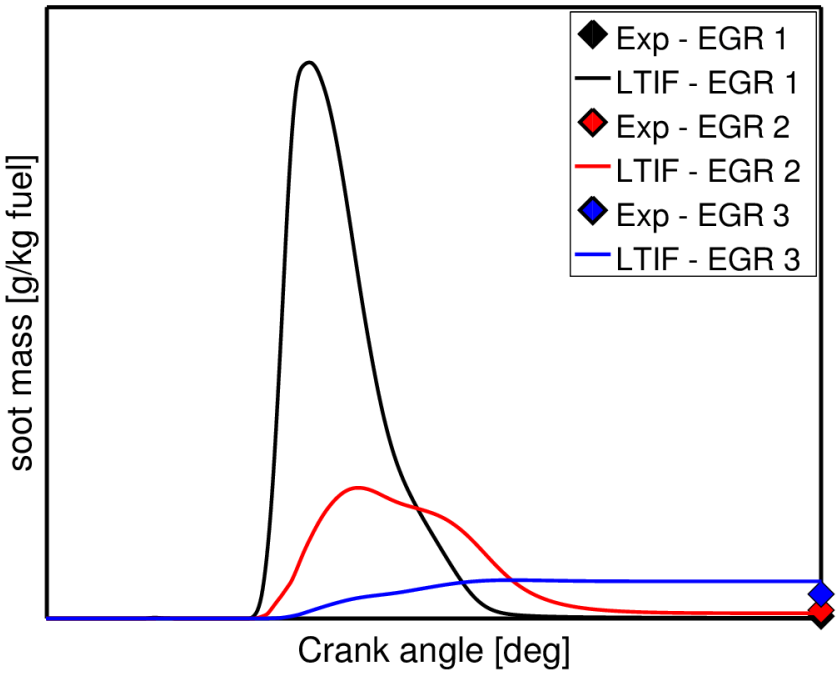




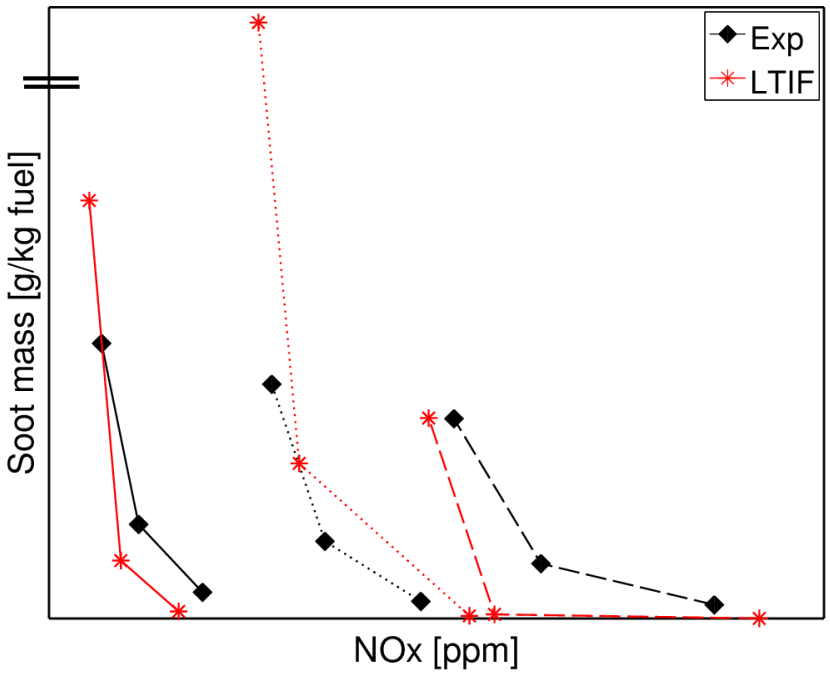
- Trends for all emissions are predicted close to the measurements

Performance soot modelling

- Soot mass over CA



- Soot-NOx-trade off



- **Effect of EGE level can be studied**
  - EGR level 1: high soot formation rate and high oxidation rate
  - EGR level 3: soot formation is limited, but at the same time less soot is oxidized

- **Predicted Soot-Nox trade off follows the measurements in terms off**
  - EGR level
  - Start of injection
- **Absolut numbers are close**

Conclusion

- LOGE TIF in CONVERGE
  - Sector cases, around 200 000 cells peak cell count)
  - Good combustion prediction is generally achieved
    - LOGE DIESEL chemistry
    - LOGE DIESEL liquid fuel database tailored for use with TIF
  - TIF benefits of the use of the CONVERGE spray models and AMR meshing strategy
    - Mixture formation
    - Automatic optimum cell size (AMR can consider variables such as mixture fraction and its variance, and flamelet markers)
- FSM
  - cell local source term library soot model with parameterized shapes for moments **predicts soot very well**

- *Computational time: DELL Precision 7810 workstation (2 x 10 cores Intel Xeon E5-2670v2 @ 2.5GHz) released July 2013. Wall clock simulation time was 7.8 hours.*

Acknowledgements

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