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Advanced Combustion Modeling with STAR-CD using Transient Flamelet Models: TIF and TFPV

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Outline

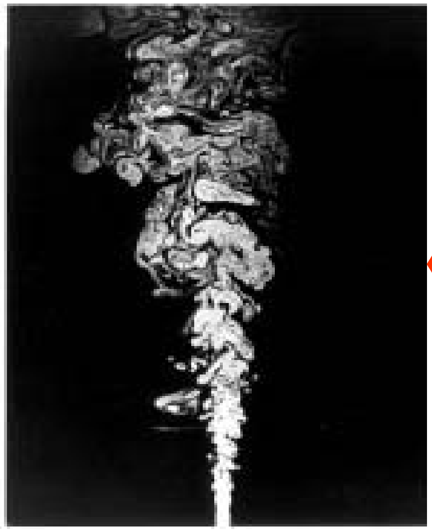
- Introduction
- General aspects of the flamelet model
- TIF: Transient interactive flamelet model
- TFPV: Transient flamelet progress variable model
- Summary and conclusions

Challenges in CFD engine modeling

- The flow is turbulent
  - Turbulence modeling required
- Spray injection and evaporation occurs
  - Spray modeling is required
- Autoignition, combustion, pollutant formation chemistry
  - Kinetic modeling required for various fuels
  - Soot, NOx models required
- ***Acceptable CPU time!***

Multidimensional modeling of turbulent reactive flow

Turbulent flowfield



Navier-Stokes equations

Combustion

?

Multidimensional modeling of turbulent reactive flow

One possible solution:

Turbulent flowfield

Navier-Stokes equations

Combustion

Flamelet modeling

- Interactive flamelet
- Transient flamelet library

General aspects of the flamelet model

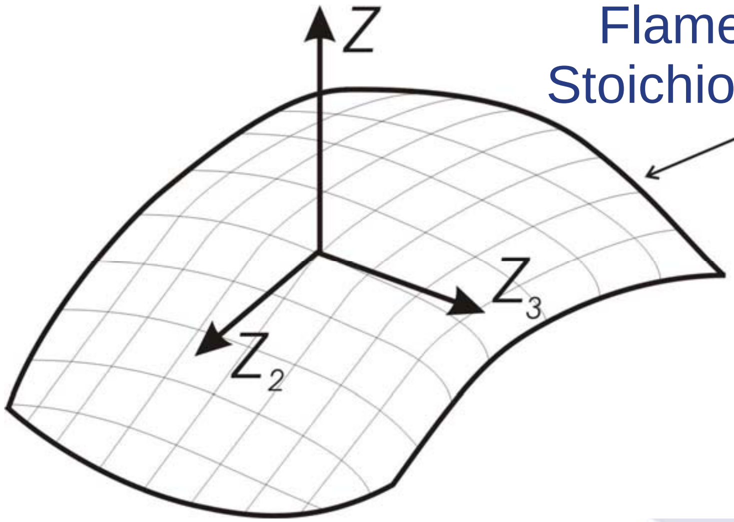
- Problem:
  - Computing transient turbulent flame configurations (e.g. ignition and combustion in Diesel engines) with detailed chemistry efficiently
  - Account for turbulence and sub-grid scale effects on chemistry in a consistent manner

- Solution:
  - Decouple chemistry and flow
  - View the flame as an ensemble of flamelets
  - Let the flamelets interact with the turbulent flowfield

General aspects of the flamelet model

Physical Coordinates $\Rightarrow$ Mixture fraction coordinate Z_i

$$t, x_1, x_2, x_3 \rightarrow \tau, Z, Z_2, Z_3$$



Flame: Surface of Stoichiometric mixture

General aspects of the flamelet model

Flamelet parameters

Mixture fraction *Z*

- Reactive scalars are a unique function of Z
- Z = 0 : Pure oxidizer
- Z = 1 : Pure fuel

Scalar dissipation χ

- Diffusion rate in mixture fraction space
- Reflects the flow field influence on chemistry

General aspects of the flamelet model

Transport of a generic scalar

$$\rho\frac{\partial\psi}{\partial t}+\rho v\frac{\partial\psi}{\partial x}-\rho D\frac{\partial^2\psi}{\partial x^2}=S_\psi$$

$$\chi=2D\left(\frac{\partial Z}{\partial x}\right)^2$$

Def. Scalar dissipation rate

Flamelet transform:

$$\begin{cases}\frac{\partial\psi}{\partial t} = \frac{\partial\psi}{\partial\tau}+\frac{\partial Z}{\partial t}\frac{\partial\psi}{\partial Z}\\ \frac{\partial\psi}{\partial x} = \frac{\partial Z}{\partial x}\frac{\partial\psi}{\partial Z}\\ \frac{\partial\psi}{\partial x_k} = \frac{\partial\psi}{\partial Z_k}+\frac{\partial Z}{\partial x_k}\frac{\partial\psi}{\partial Z}, k=2,3\end{cases}$$

Equations in flamelet space

$$\rho\frac{\partial\psi}{\partial\tau}=\rho\frac{\chi}{2}\frac{\partial^2\psi}{\partial Z^2}+S_\psi-R(\psi)$$

$$R(\psi)=\rho v\frac{\partial\psi}{\partial Z}+\frac{\partial}{\partial x}\left(\rho D\frac{\partial\psi}{\partial Z}\right)-\rho D\sum_{k=2}^{3}\left(\frac{\partial Z}{\partial x_k}\frac{\partial^2\psi}{\partial Z\partial Z_k}+\frac{\partial^2\psi}{\partial Z_k{}^2}\right)$$

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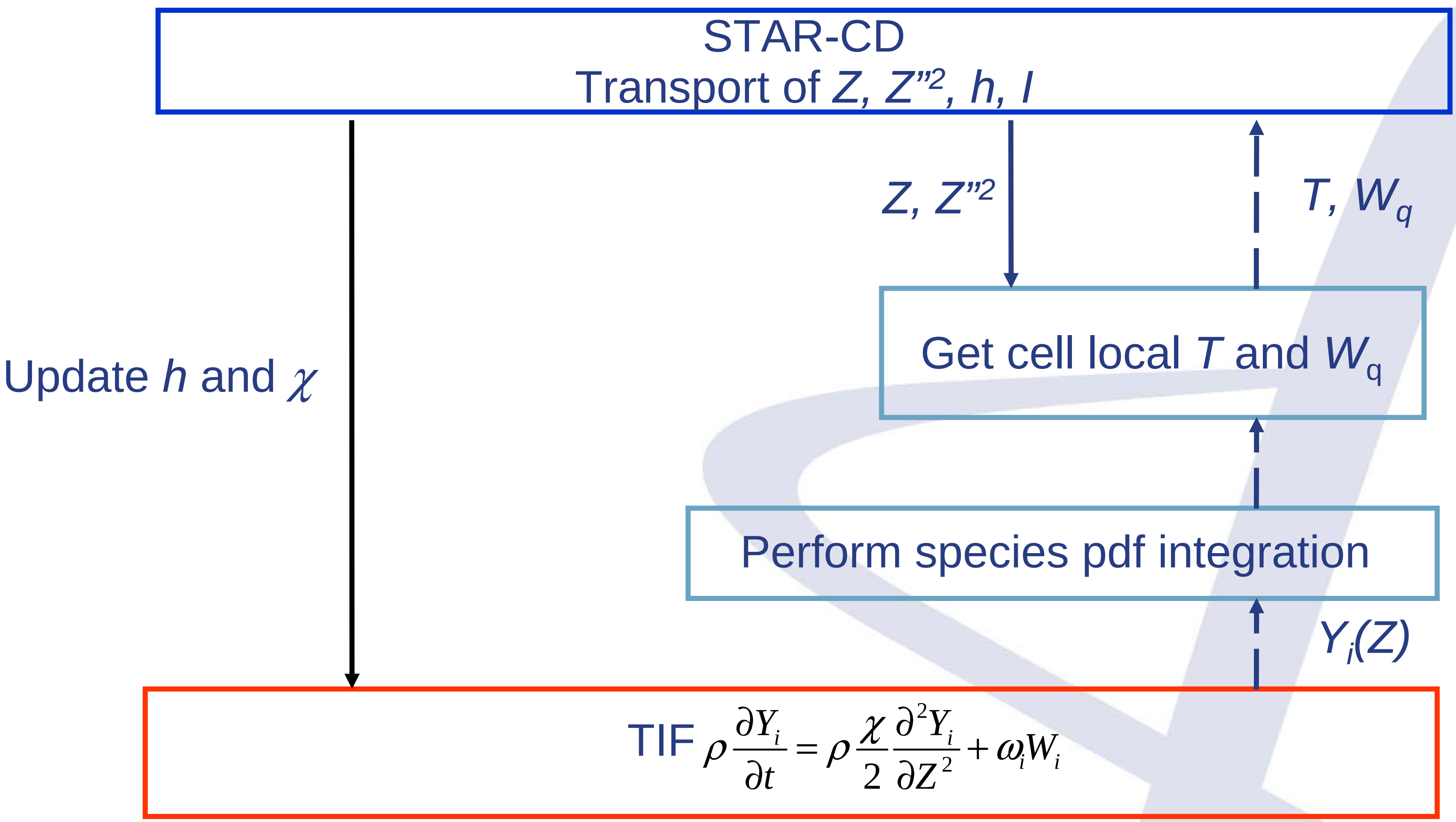
TIF – Transient Interactive Flamelet

- Transient flamelet calculations performed **on-line** with the flow calculation
- Detailed chemistry calculation performed by the TIF solver
- Arbitrary number of TIF flamelets can be used to discretize the computational domain
- Flamelet discretization based on evaporated fuel mass amount
- New flamelets inherit the state of the previous flamelet, but get their own scalar dissipation rate history
- For multiple injections, a three-zone mixing model treatment is applied

STAR-CD – TIF coupling



TIF Engine Calculation – Engine Data

Swept volume	0.6 L
Compression ratio	17
Number of nozzle holes	7
Nozzle hole diameter	0.15 mm
Speed	2000 rpm
Fuel type	Diesel
Fuel amount	12.5 mg
Start of injection	Varying
EGR ratio	Varying, Base case 0 %

5 Flamelets used

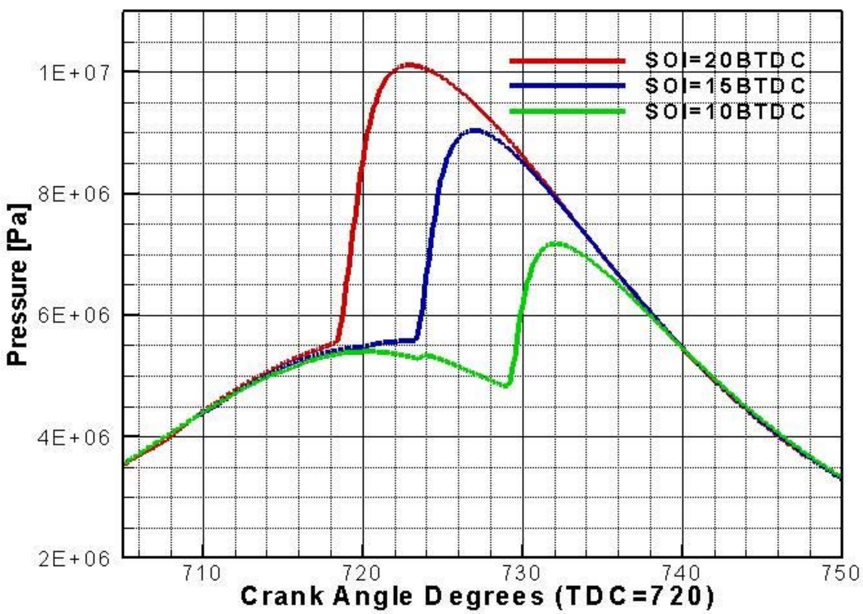
Timing of generating a new flamelet based on the evaporation process

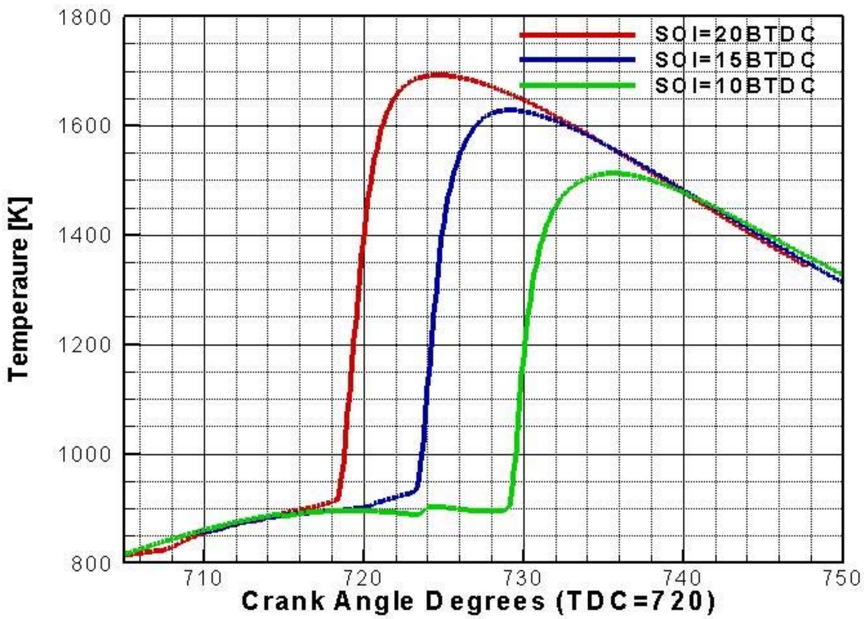
A chemistry for diesel with 101 species and 841 reactions used

TIF Engine Calculation – 0 % EGR, varying SOI

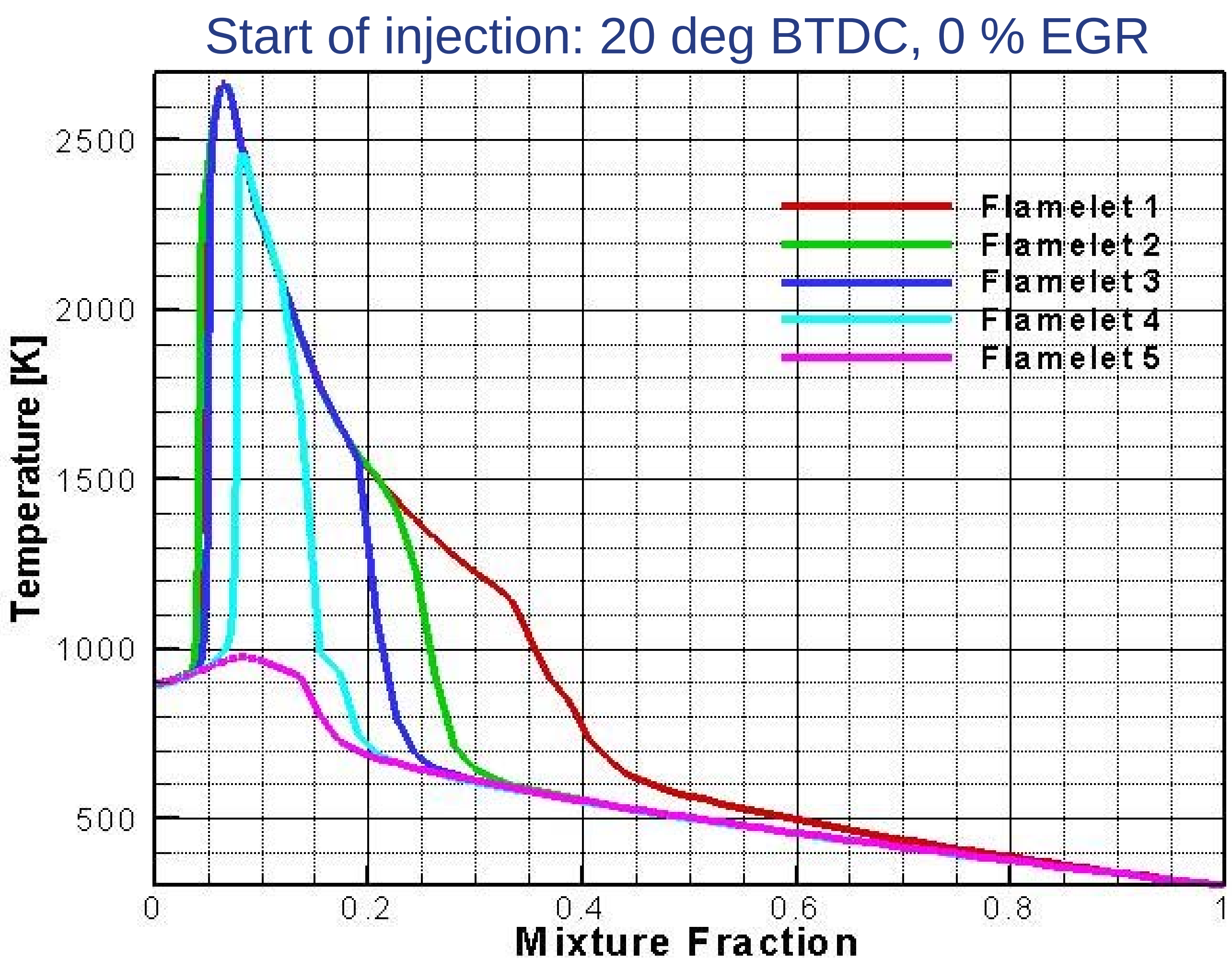
Variation of injection timing

Start of injection: 20 deg BTDC, 15 deg BTDC, 10 deg BTDC
0 % EGR





TIF Engine Calculation – Flamelet Temperature CA 718.5



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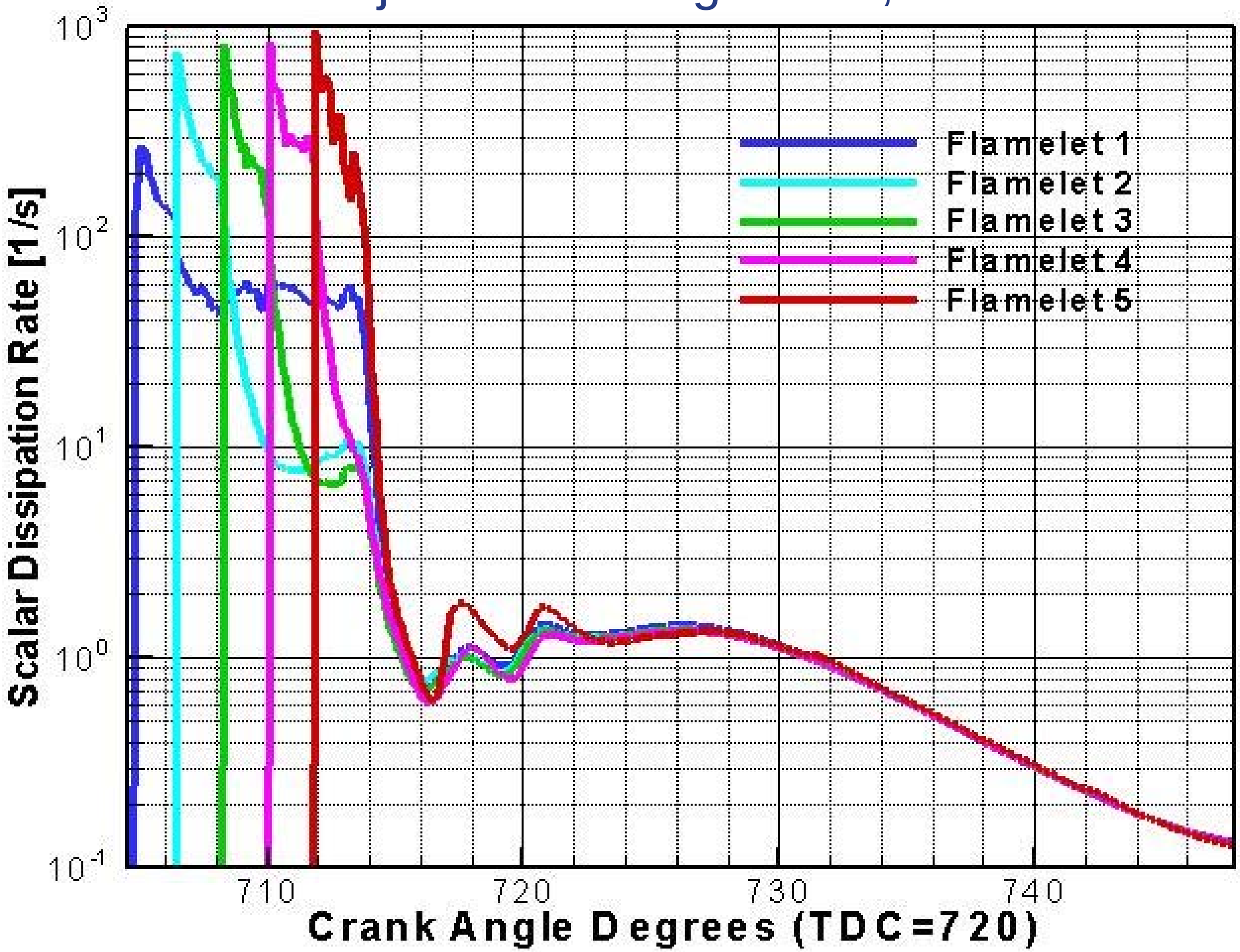
TIF Engine Calculation – Scalar Dissipation Rate

Start of injection: 20 deg BTDC, 0 % EGR



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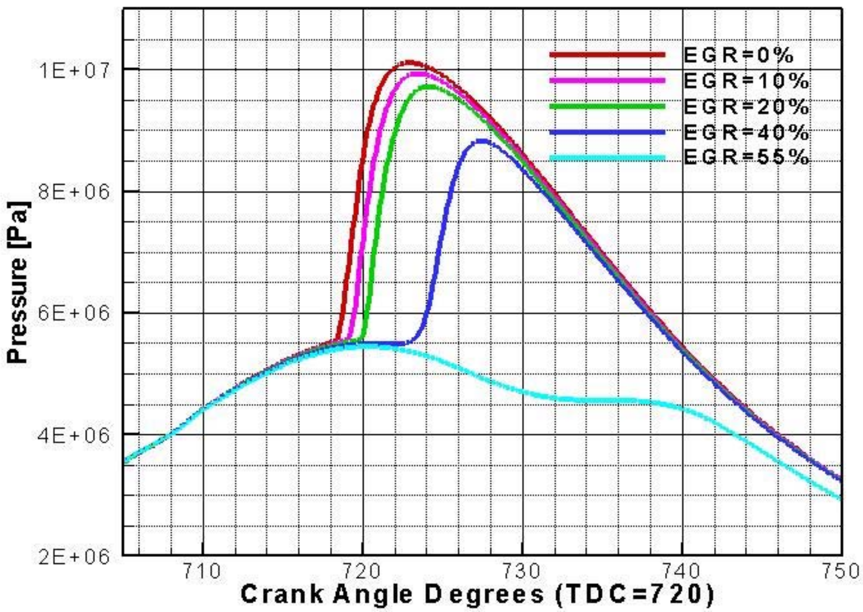
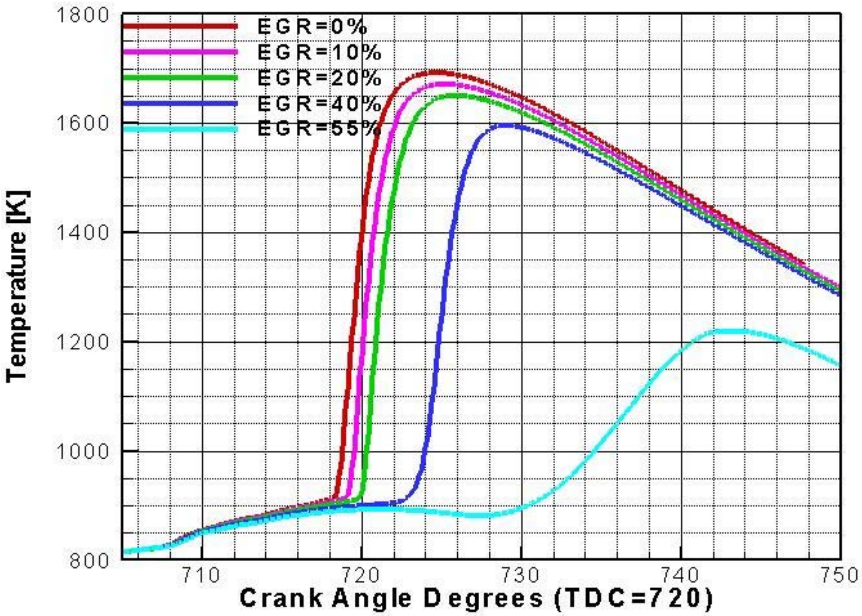
TIF Engine Calculation – EGR Sensitivity Study

Variation of EGR amount

Start of injection: 20 deg BTDC
EGR: 0 %, 10 %, 20 %, 40 %, 55 %





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TIF – Summary

- The TIF coupling to STAR-CD was presented
  - Transport of mixture fraction, mixture fraction variance, and flamelet probability
  - Discretization of computational domain in arbitrary number of flamelets
  - Fully parallel treatment

- Sample calculations have been carried out.
- The TIF model is able to produce anticipated trends
  - Start of injection effects
  - EGR effects

TFPV - Transient flamelet progress variable model

- The transient ignition process of flamelets is tabulated for a wide range of conditions
- The precomputed transient flamelet library is called from STAR-CD for each cell
- The transient flamelet library allows for accounting for the *cell local flamelet state when determining the fate of the combustion process*

TFPV - Transient flamelet progress variable model

- Progress variable defined using chemical enthalpy integrated over the flamelet

$$C = \frac{\int_0^1 \sum_{i=1}^{N_s} h_{298,i}(Y_i(Z),\tau)dZ - \int_0^1 \sum_{i=1}^{N_s} h_{298,i,u}(Y_i(Z),0)dZ}{\int_0^1 \sum_{i=1}^{N_s} h_{298,i,b}(Y_i(Z),\tau_\infty)dZ - \int_0^1 \sum_{i=1}^{N_s} h_{298,i,u}(Y_i(Z),0)dZ}$$

Transport eqn for chemical enthalpy

$$\rho\frac{\partial h_{298}}{\partial t} + \rho v_\alpha \frac{\partial h_{298}}{\partial x} - \rho D \frac{\partial^2 h_{298}}{\partial x_\alpha^2} = \sum_{i=1}^{N_s} \omega_i h_{i,298}$$

Transform to Z – C space

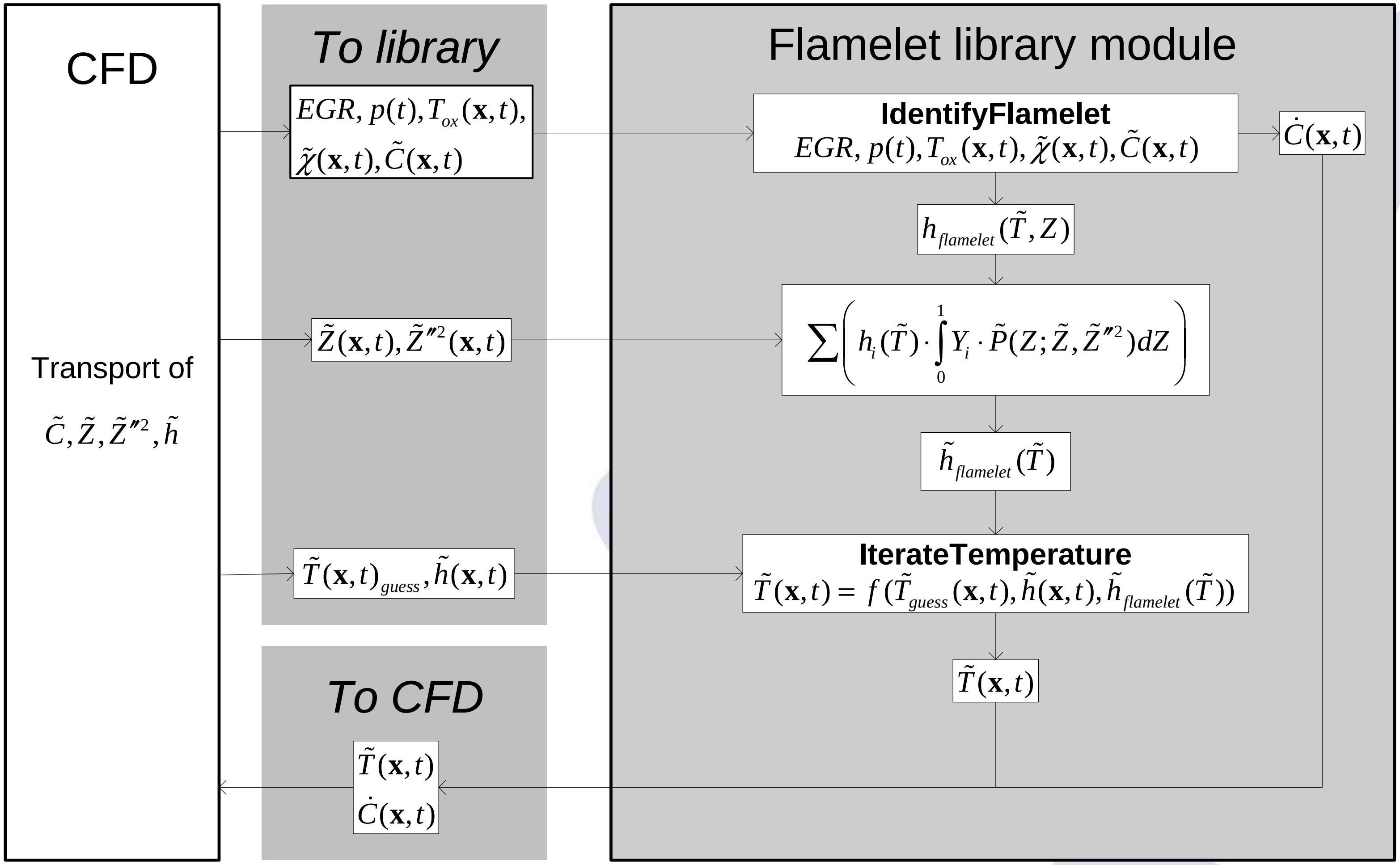
$$\begin{cases} \frac{\partial \psi}{\partial t} = \frac{\partial \psi}{\partial Z}\frac{\partial Z}{\partial t} + \frac{\partial \psi}{\partial C}\frac{\partial C}{\partial t} + \underline{\frac{\partial \psi}{\partial t}} \\ \frac{\partial \psi}{\partial x_\alpha} = \frac{\partial \psi}{\partial Z}\frac{\partial Z}{\partial x_\alpha} + \frac{\partial \psi}{\partial C}\frac{\partial C}{\partial x_\alpha} \end{cases}$$

Transport eqn for the progress variable

$$\rho\frac{\partial C}{\partial t} + \rho v_\alpha \frac{\partial C}{\partial x_\alpha} - \rho D \frac{\partial^2 C}{\partial x_\alpha^2} = \rho \dot{C} - \frac{\rho}{\partial h_{298}/\partial C}\underline{\frac{\partial h_{298}}{\partial t}}$$

H Lehtiniemi, F Mauss, M Balthasar and I Magnusson, Combust Sci and Tech 178 (10-11) 2006 1977-1997

TFPV – Coupling to STAR-CD



TFPV – Sample engine calculation

Swept volume		2.0 L
Compression ratio		15.3
Number of nozzle holes		6
Nozzle hole diameter		0.2 mm
Speed		1176 rpm
Fuel type		Diesel
Fuel amount		74.35 mg
λ		1.24
Start of injection		361 CA
EGR ratio		0.32

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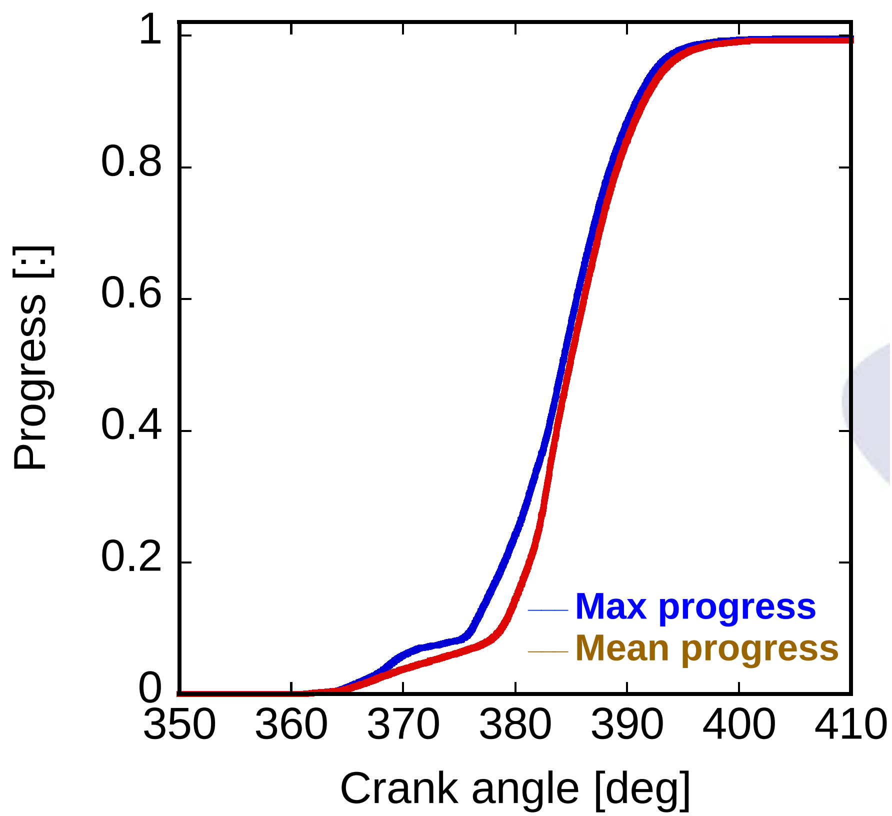
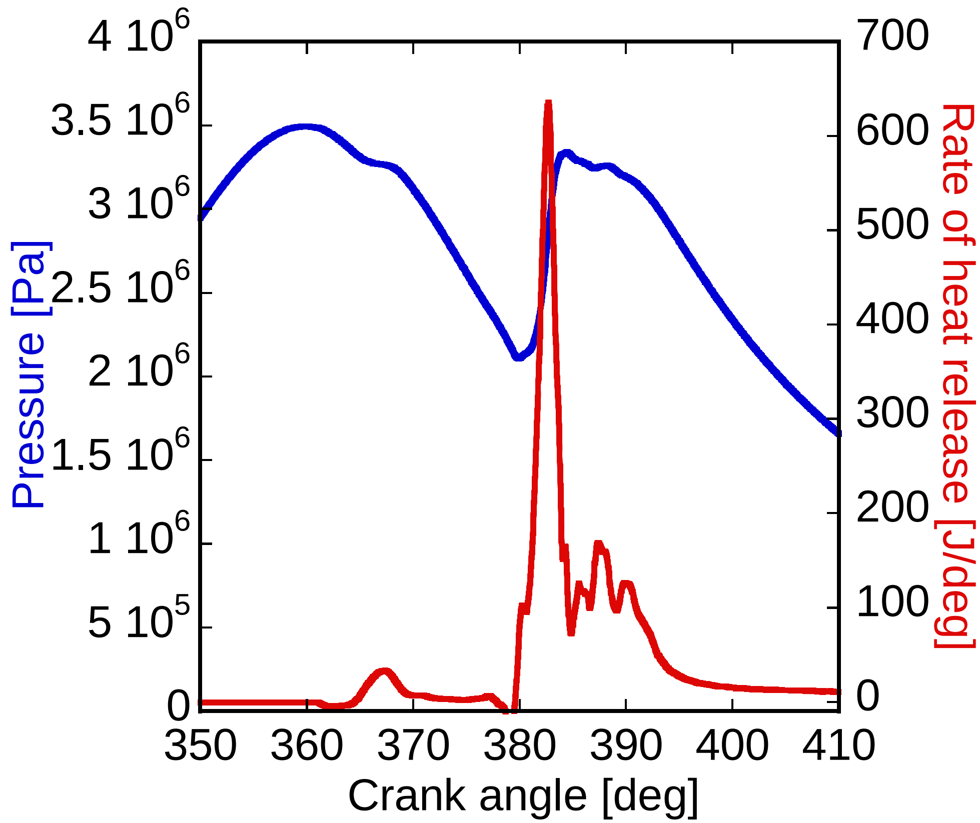
TFPV – Sample engine calculation

Combustion progress



Pressure and rate of heat release



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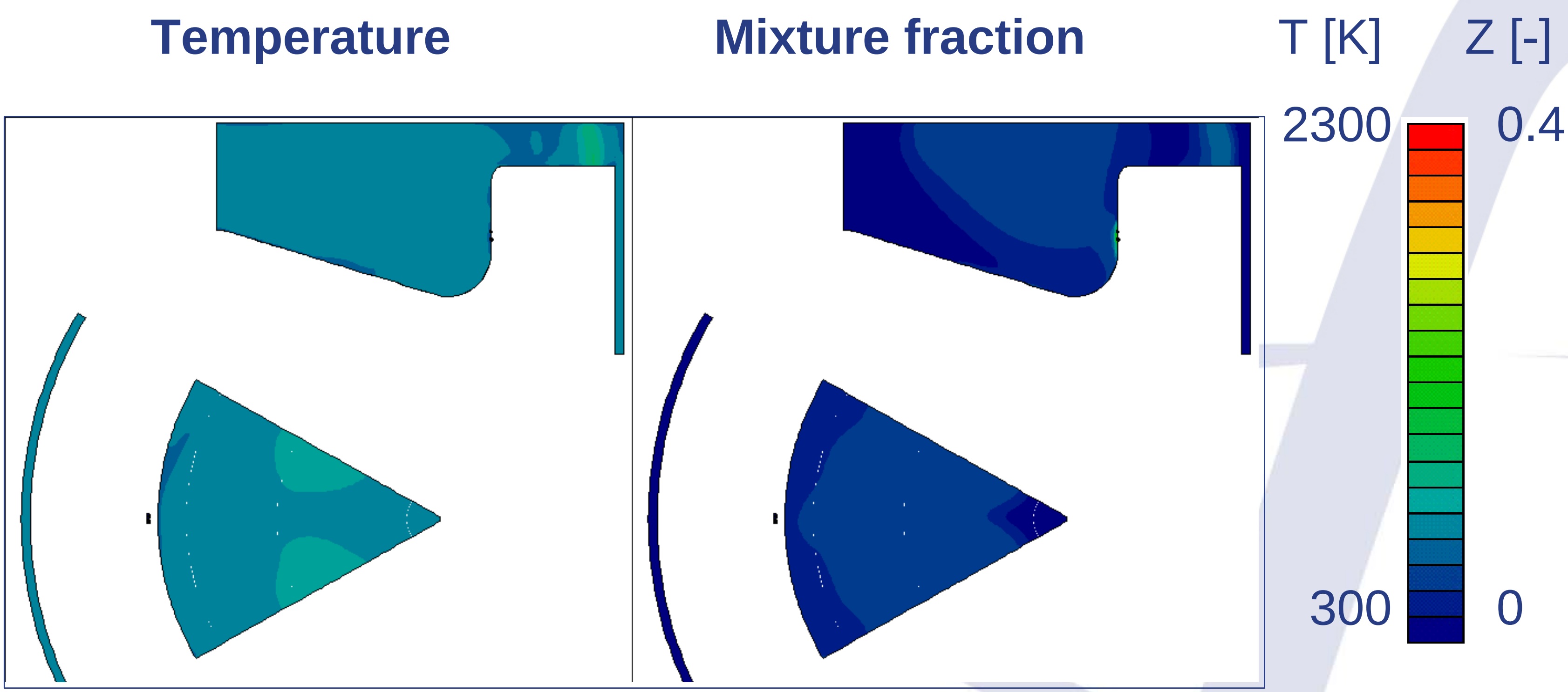
TFPV – Sample engine calculation CA 380



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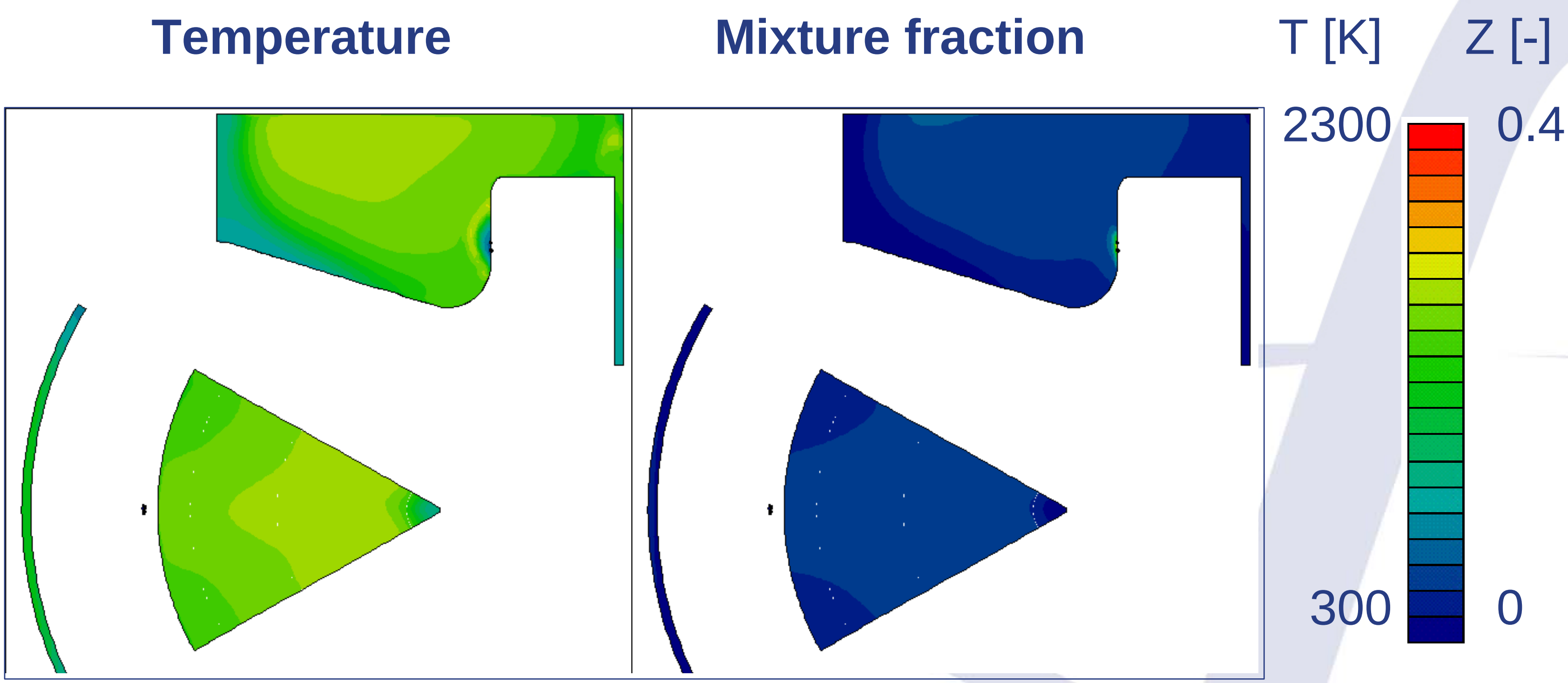
TFPV – Sample engine calculation, CA 385



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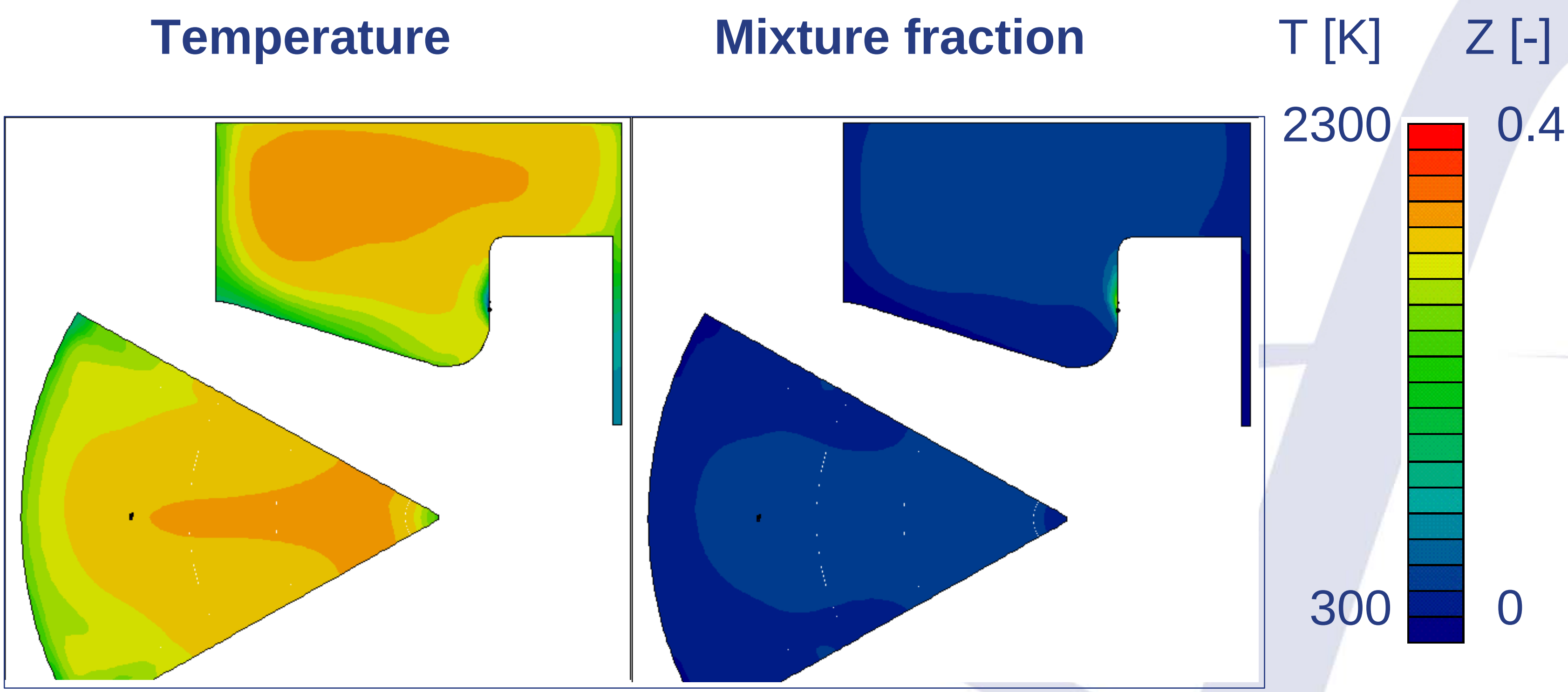
TFPV – Sample engine calculation, CA 395



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TFPV - Summary

- The TFPV coupling to STAR-CD was presented
  - Transport of mixture fraction, mixture fraction variance, and progress variable
  - Local effects of turbulence (scalar dissipation rate) and heat losses can be accounted for on a cell level
  - Fully parallel treatment

- A TFPV sample calculation was presented
  - Low load, 32 % EGR with long delay before main ignition

Summary and Conclusion

- The TIF model allows for
  - Efficient treatment of chemistry
  - Consistent handling of turbulence interactions
  - Efficient treatment of complex soot and emission chemistry
  - Fully parallel simulations
- The TFPV model allows for
  - Consideration of effects of local inhomogeneities and local variations of scalar dissipation rate on the chemistry
  - Arbitrary large chemistry can be used in the tabulation without influencing the CFD simulation CPU time
  - Coupling to library based emission models
  - Fully parallel simulations
- Sample 3D CFD simulations using both models have been presented