Assessment of various combustion modelling approaches and validation by means of data from a large marine engine reference experiment

32nd IEA Task Leader Meeting,
Nara, Japan, Jul. 2010

Michele Bolla[*], Yuri M. Wright[*,†] and Konstantinos Boulouchos[*],
Kai Herrmann[‡] and Beat von Rotz [‡]

[*] Aerothermochemistry and Combustion Systems Laboratory, ETH Zürich, Switzerland
[‡] Wärtsilä Switzerland, Ltd.

[†]mailto:wright@lav.mavt.ethz.ch

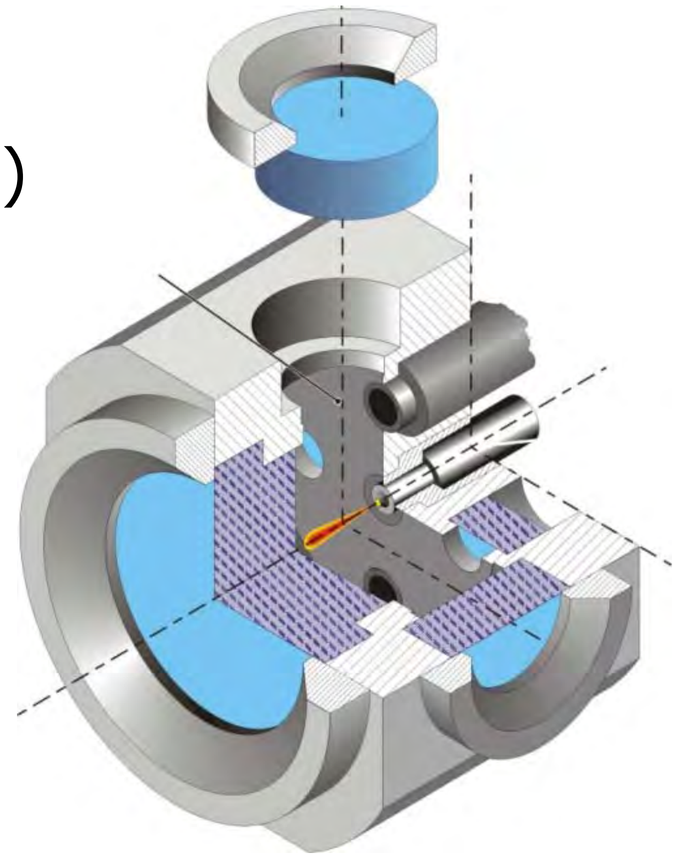
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Outline

- Introduction to ‚generic‘ spray test rigs
- Particulars of large marine engine reference experiment
- Overview of the numerical model
- Combustion models for spray combustion
- First results
- Conclusions
- Outlook

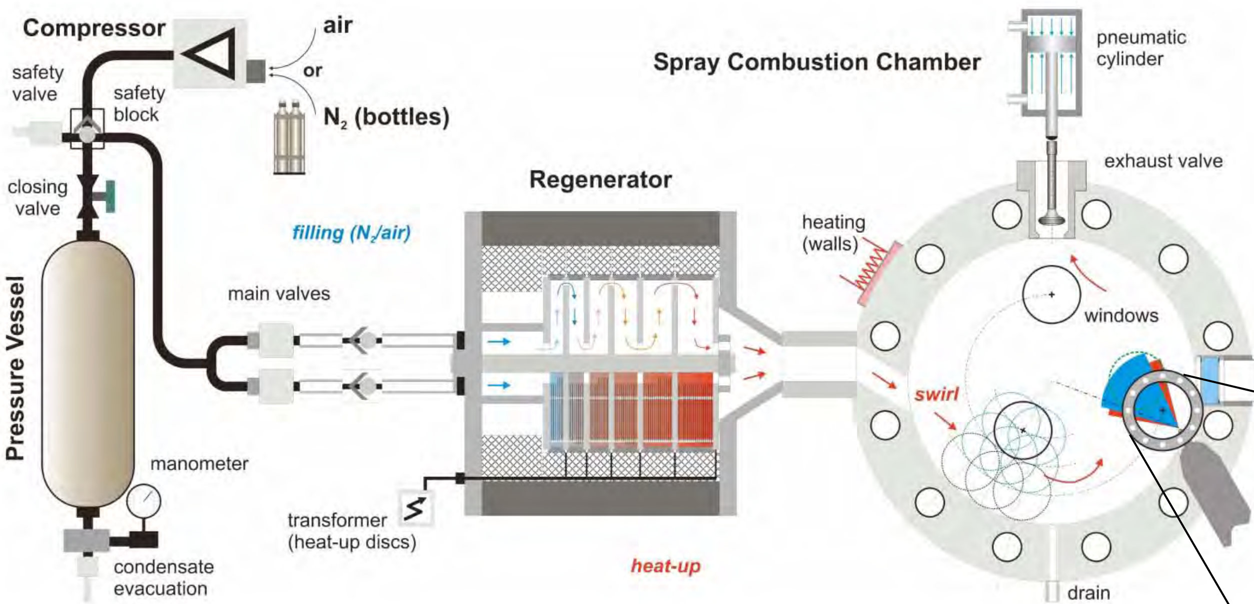
‚Classical' spray test rigs

- Large body of literature (both experiment and simulation)
- Volume ~0.5-2.0 litres (~100mm diam.)
- Constant volume/pressure chambers
- Good optical access
- Initial conditions around:
  - ~800K, 80 bar (electric heaters)
  - >1100K (with pre-combustion)
  - quiescent /homogeneous turbulence
- Central fuel injector (single/multiple)



Source: Schneider, PhD Thesis ETH No. 15004 (2003)

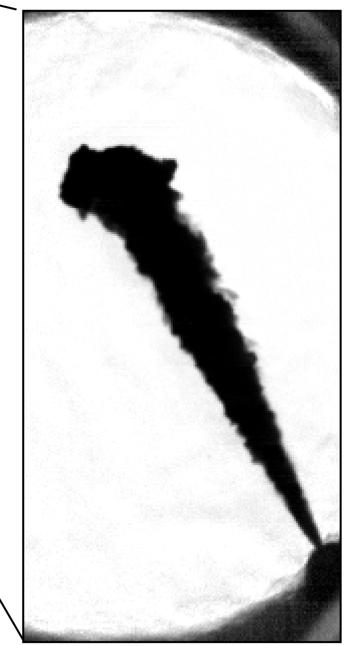
Large marine engine reference experiment



Source: Herrmann et al., CIMAC 2007

Chamber dimension
D = 500 mm
H = 150 mm

Shadow-image



conditions at start of injection

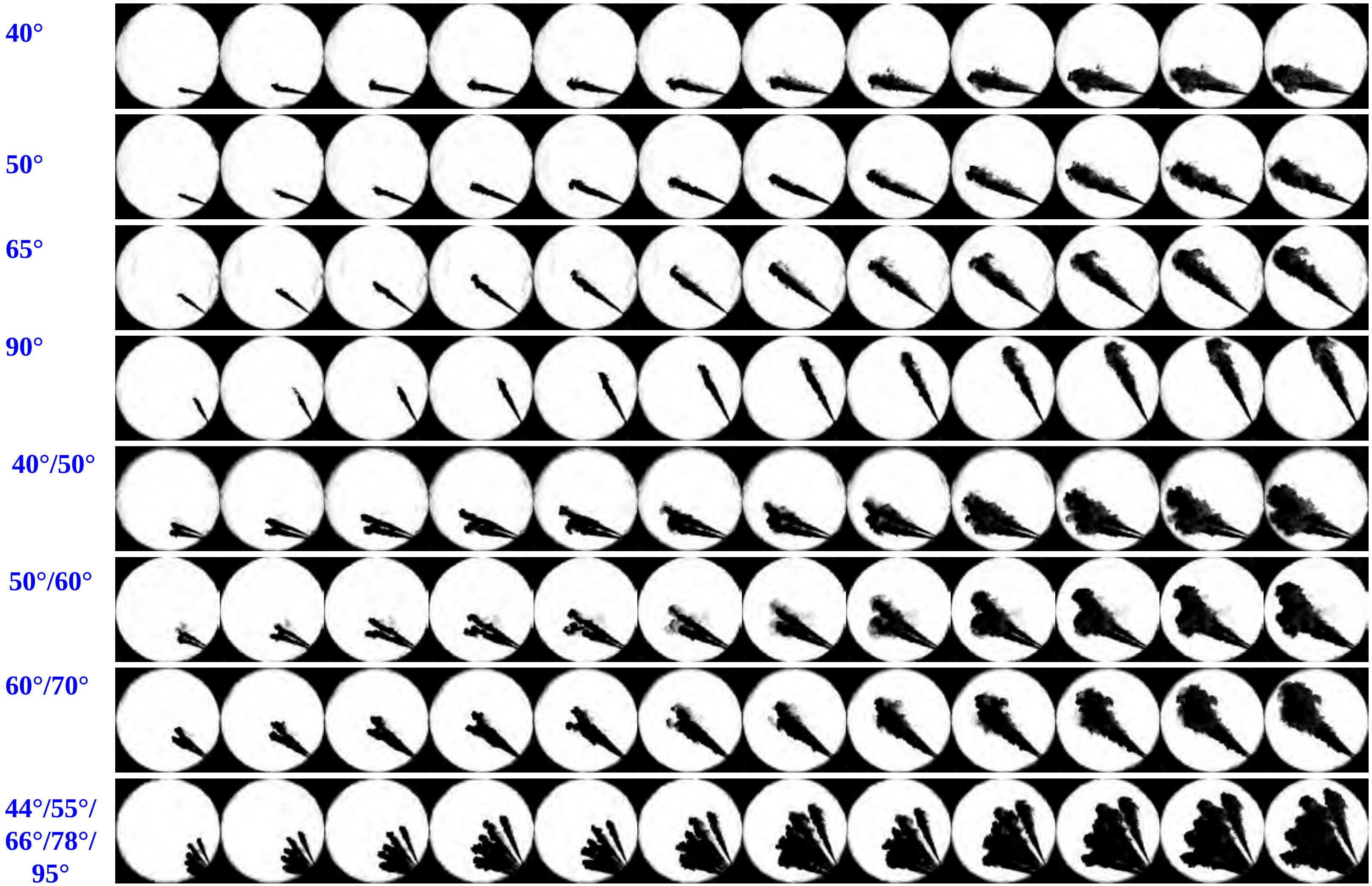
- P ≈ 100...130 bar
- T > 900 K
- high swirl level: $U_{tan\ max}$ =15...25 m/s
- peripheral fuel injection
- Various fuel qualities: Diesel, to heavy fuel oil (HFO)

Source: Herrmann, Kyrtatos, Schulz, Weisser, von Rotz, Schneider & Boulouchos., ICLASS (2009)

Experimental data-sets (examples)

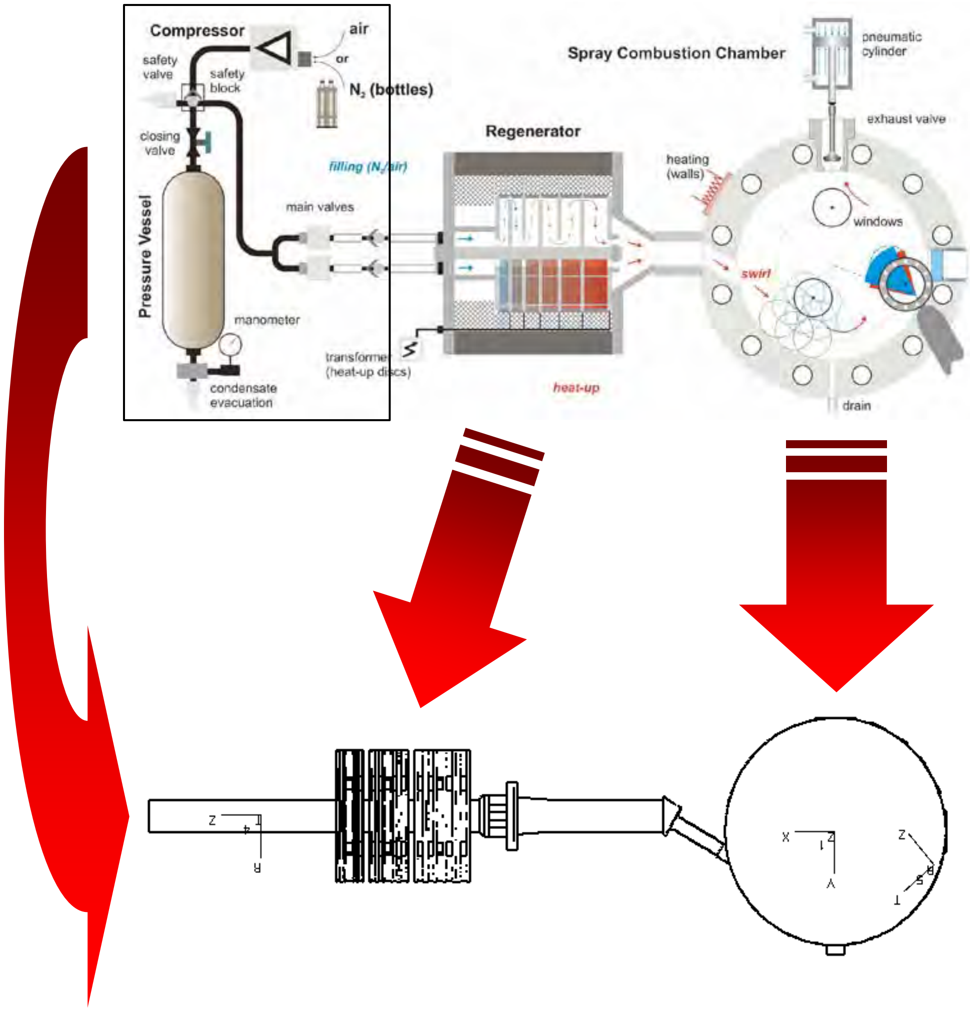
Impressions measurement campaigns (M08/M09)

9 MPa / 900 K



Source: Herrmann, von Rotz, Schulz, Weisser, Boulouchos, Schneider, ILASS 2010

Numerical set-up

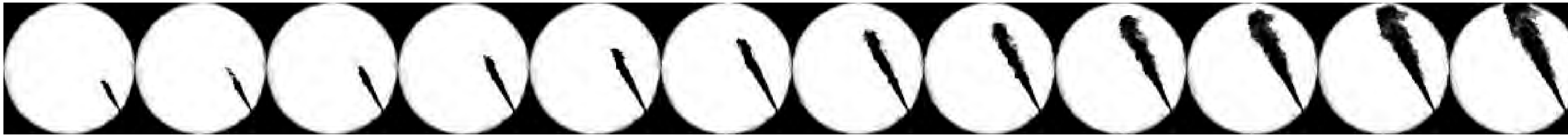


- **3D CFD code STAR-CD v4.12**
- **Geometry with 816k Cells**
  - Orifice resolution in near nozzle region
- **Initial conditions from full blow-down simulation**
- **Turbulence model: κ-ε-RNG**
- **Spray model:**
  - Atomisation: Huh
  - Break-up: Reitz-Diwakar
- **Various combustion models**
  - EBU LaTCT
  - ECFM-3Z
  - Conditional Moment Closure

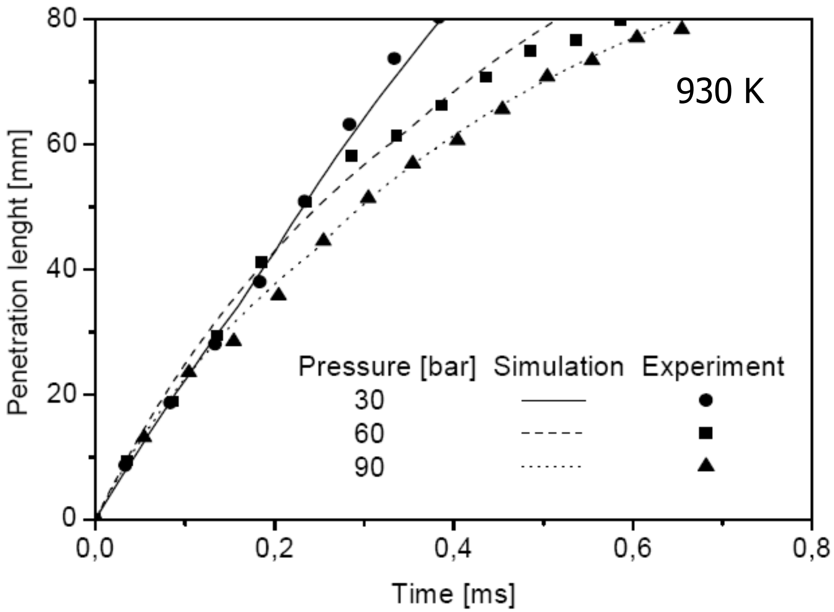
Source: Herrmann et al., CIMAC 2007

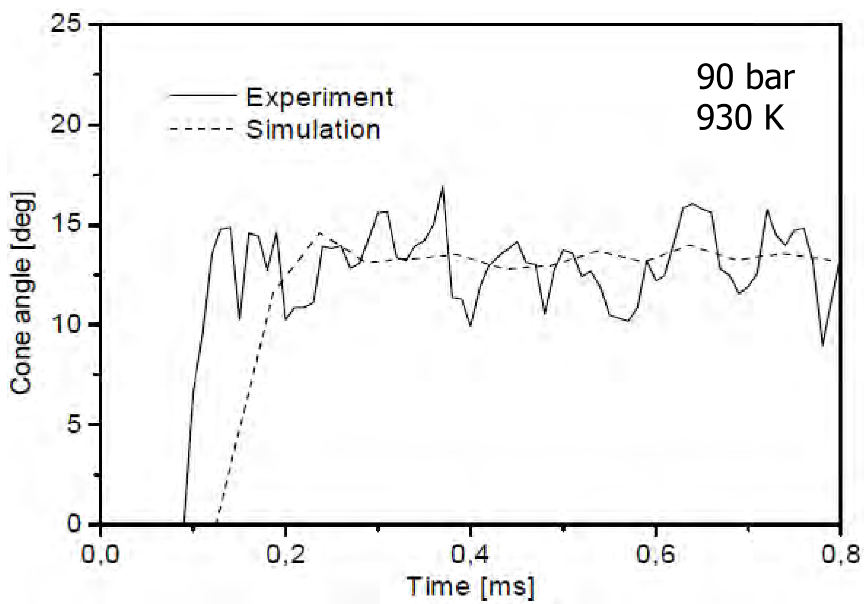
Spray validation (IEA TLM 2009)

- **One reference set chosen for single-orifice nozzle**



- Spray model constant tuned for reference condition
- Good agreement for penetration/cone angle for three pressure levels
- Further validation data yet to come (drop sizes and velocities)





Source: Schulz et al., CIMAC 2010, Paper 247

Next: Assess three combustion models

- **First assessment**
- **Three ‚families' of models chosen:**

Eddy break-up	**ECFM-3Z**	**Conditional Moment Closure (CMC)**

▪ 'simple' model
▪ Inexpensive
▪ In many CFD codes
▪ Requires model constant tuning
	▪ Wide-spread model in industrial CFD
	▪ 'affordable'
	▪ More physics
		▪ Research code
		▪ Computationally demanding
		▪ 'complex' model
		▪ Demonstrated for different setups:
		  ▪ Aachen bomb
		  ▪ ETH bomb
		  ▪ Heavy-duty engine

All 'small' compared to marine engines!
Performance for large dimensions/time-scales?

The Eddy break-up model

- **Species conservation**

$$\rho \frac{\partial \tilde{Y}_i}{\partial t} + \rho \mathbf{v} \cdot \nabla \tilde{Y}_i - \nabla \cdot (\rho D_i \nabla \tilde{Y}_i) = \dot{\omega}_i \quad \textit{where} \quad \dot{\omega} = \prod_{k=1}^{n} c_k^{\nu'_k} A T^b \exp\left(-\frac{E}{RT}\right)$$

$$T = \tilde{T} + T''$$

$$\frac{E}{RT} = \frac{E}{R\tilde{T}} + \frac{ET''}{R\tilde{T}^2} + \ldots \qquad \textit{but} \quad \frac{E}{R\tilde{T}} > 10 \quad \textit{and} \quad \frac{T''}{\tilde{T}} \approx 0.1..0.3$$

Source:
Peters (2000)

- **'Available' in many CFD codes (e.g. STAR, KIVA, ...)**

$$\frac{\partial Y_m}{\partial t} = -\frac{Y_m - Y_m^*}{\tau_c}$$

„Relax to equilibrium with a characteristic time"
Spalding, Magnussen, Kong, Reitz, ...

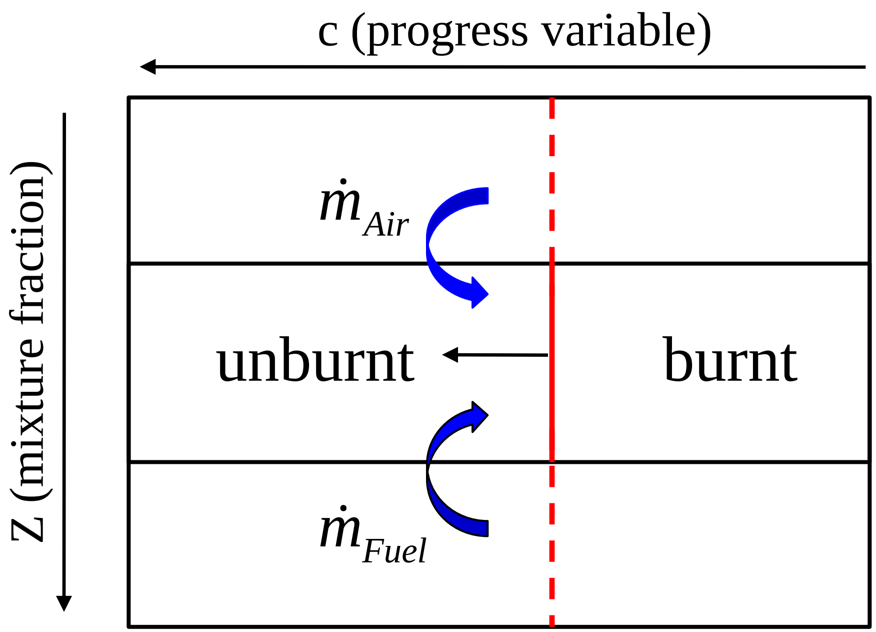
$$\frac{1}{\tau_l} = 2 \cdot 10^{10} \cdot \left[C_{14}H_{30}\right]^{0.25} \left[O_2\right]^{1.5} \exp\left(-\frac{E}{RT}\right) \qquad \textit{and} \qquad \tau_t = C_2 \frac{\varepsilon}{k}$$

$$\tau_c = \tau_l + f\,\tau_t$$

$$\overline{\dot{\omega}_F} = -\frac{\rho \boxed{A}}{\tau_C} MIN\left(Y_F, \frac{Y_O}{\nu}, B\frac{Y_P}{1+\nu}\right)$$

Assume this is 'known' – when do we 'switch it on' ?

Extended Coherent Flame Model (ECFM-3Z)



Air $$\dot{m}_{Air} = \frac{\rho}{\tau_{turb}} Y_{Air}\left(1 - Y_{Air}\left(\frac{\rho W_{Mixed}}{\rho^u W_{Air}}\right)\right)$$

Mixing layer $$\dot{\omega}_{CFM} = -\rho_u s_L \Sigma$$

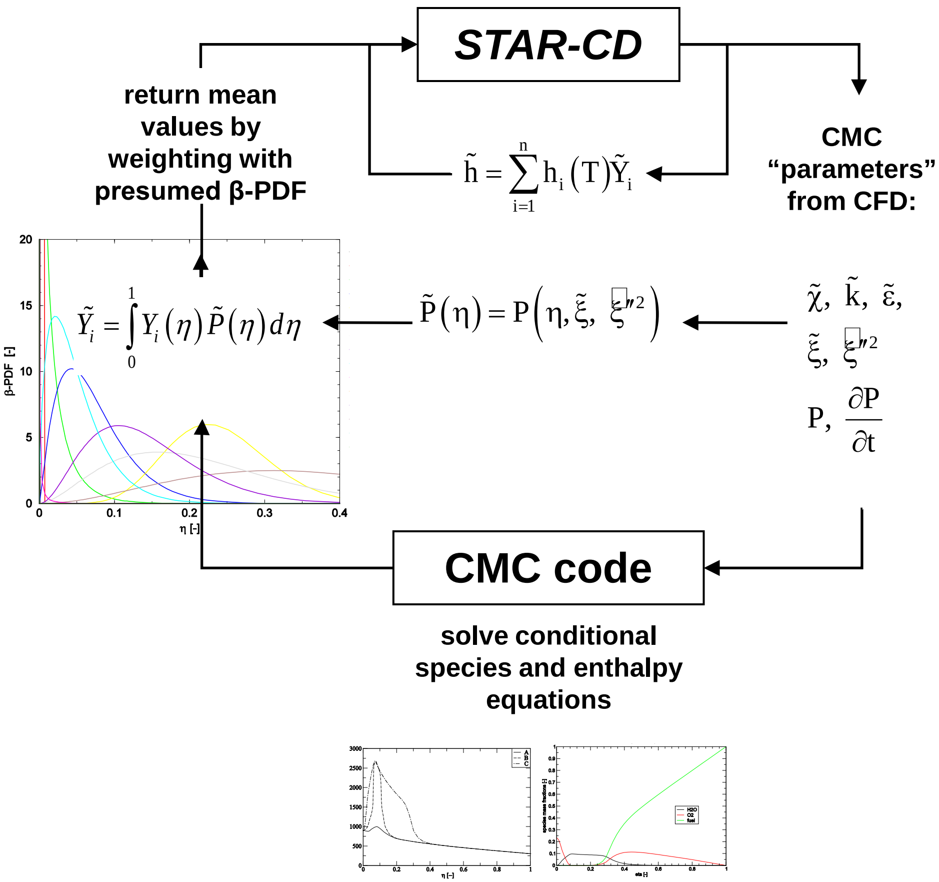
Fuel $$\dot{m}_{Fuel} = \frac{\rho}{\tau_{turb}} Y_{Fuel}\left(1 - Y_{Fuel}\left(\frac{\rho W_{Mixed}}{\rho^u W_{Fuel}}\right)\right)$$

- Each cell is divided into 3 zones (3Z)
- Ignition from tabulated n-Heptane chemistry
- Flame surface density equation for combustion progress
- Post-flame:
  - Species oxidation treated with EBU model
  - Chemical equilibrium/dissociation
  - NO_x (ext. Zeldovich)

Source: STAR-CD Methodology guide, v4.12
Duclos et al. Oil Gas Sci. Technol., 54 (1999)
Colin & Benkenida, Oil Gas Sci. Technol., 59 (2004)

Conditional Moment Closure (CMC)

- Interfacing STAR-CD / CMC code

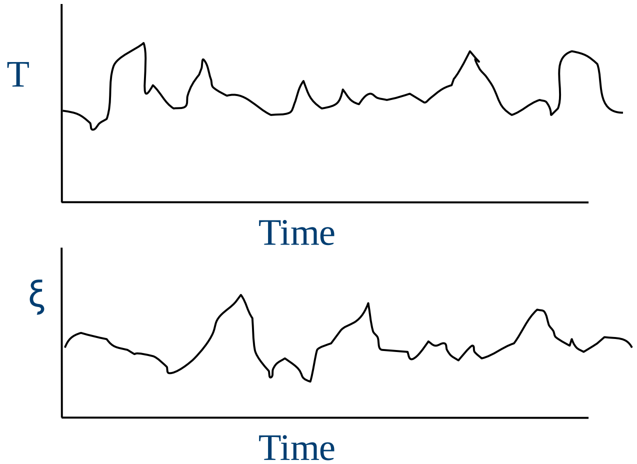


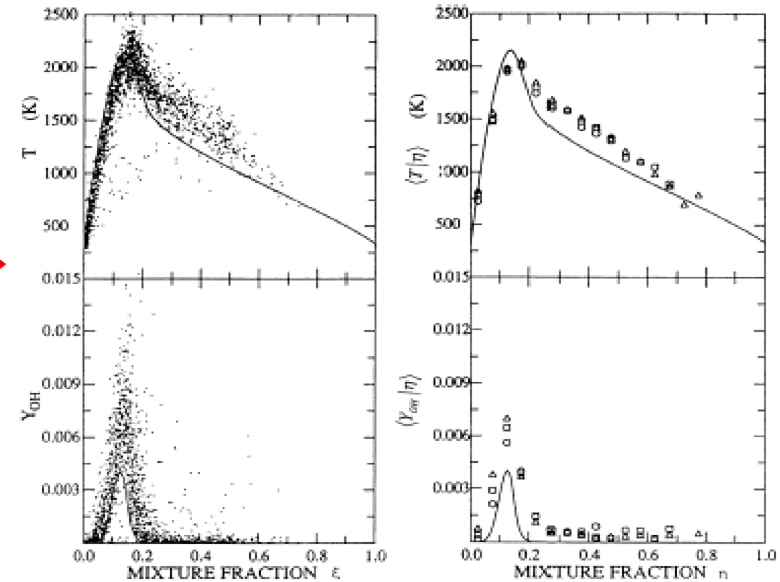
Wright, de Paola, Mastorakos & Boulouchos, Comb. Flame 143 (2005)

- Presumed PDF approach
- Full two-way coupling to STAR-CD
- Accounts for turbulence-chemistry interaction
- Solve conditional species and temperature in physical and conserved scalar space (mixture fraction)
- 'Arbitrary' chemistry possible
  - Reduced C_7H_{16} mechanism (Pitsch*, 22 species & 18 rxns)
- Operator splitting approach, parallel

*) Mechanism: Liu., Hewson, Chen & Pitsch, Comb. Flame 137 (2004)

Conditional averaging – concept





Piloted diffusion flame of methanol
Source: R.W. Bilger, Physics of Fluids (1993)

- **Conservation equations:**

$$\rho\frac{\partial Y_i}{\partial t} + \rho v\cdot\nabla Y_i - \nabla\cdot\left(\rho D_i \nabla Y_i\right) = \dot{\omega}_i$$

- **‚Bilger-approach' – consider:**

$$Y\left(\underline{x},t\right) = Q\left(\xi\left(\underline{x},t\right),\underline{x},t\right) + y'\left(\underline{x},t\right) \quad \text{where} \quad Q = \left\langle Y\left(\underline{x},t\right)\middle|\,\xi\left(\underline{x},t\right) = \eta\right\rangle$$

- **Increased dimensionality of the problem: Q(x̲,η,t)**
- **But Qs have weaker spatial dependence than unconditional values**

CMC equations: Formulation

$$Q_\alpha = \langle Y_\alpha | \xi = \eta \rangle$$

Species

$$\frac{\partial Q_\alpha}{\partial t} + \underbrace{\langle u_i | \eta \rangle \cdot \nabla Q_\alpha}_{\text{Conditional velocity}} = \underbrace{\langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2}}_{\text{Molecular mixing}} - \underbrace{\frac{\nabla \cdot \left(\langle u_i'' Y_\alpha'' | \eta \rangle \langle \rho \rangle \tilde{P}(\eta) \right)}{\langle \rho \rangle \tilde{P}(\eta)}}_{\text{Conditional turbulent flux}} + \underbrace{\langle w_\alpha | \eta \rangle}_{\text{Chemistry}}$$

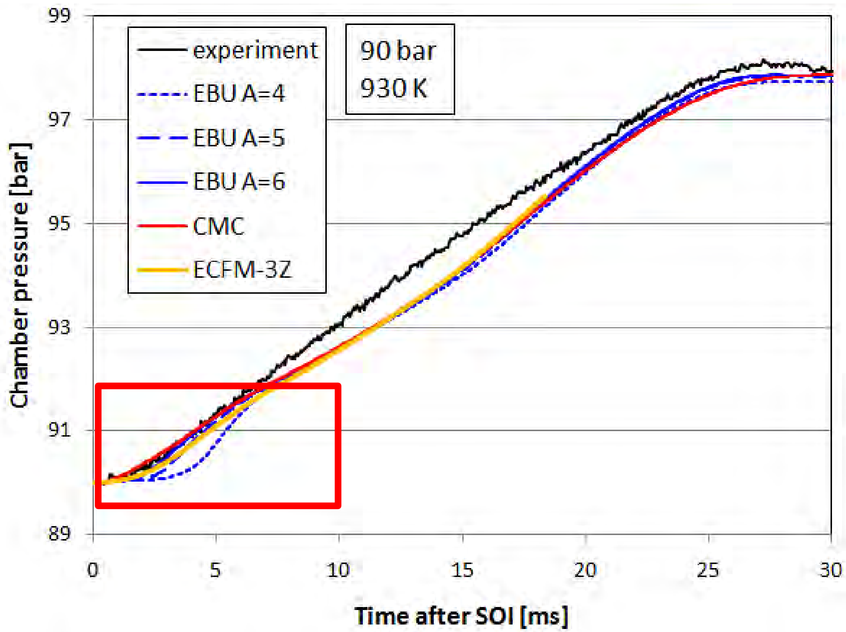
Temperature

$$\frac{\partial Q_T}{\partial t} + \langle u_i | \eta \rangle \cdot \nabla Q_T = \langle N | \eta \rangle \frac{\partial^2 Q_T}{\partial \eta^2} + \langle N | \eta \rangle \left[\frac{1}{\langle c_p | \eta \rangle} \left(\frac{\partial \langle c_p | \eta \rangle}{\partial \eta} + \sum_{\alpha=1}^{N} \langle c_{p,\alpha} | \eta \rangle \frac{\partial Q_\alpha}{\partial \eta} \right) \right] \frac{\partial Q_T}{\partial \eta}$$

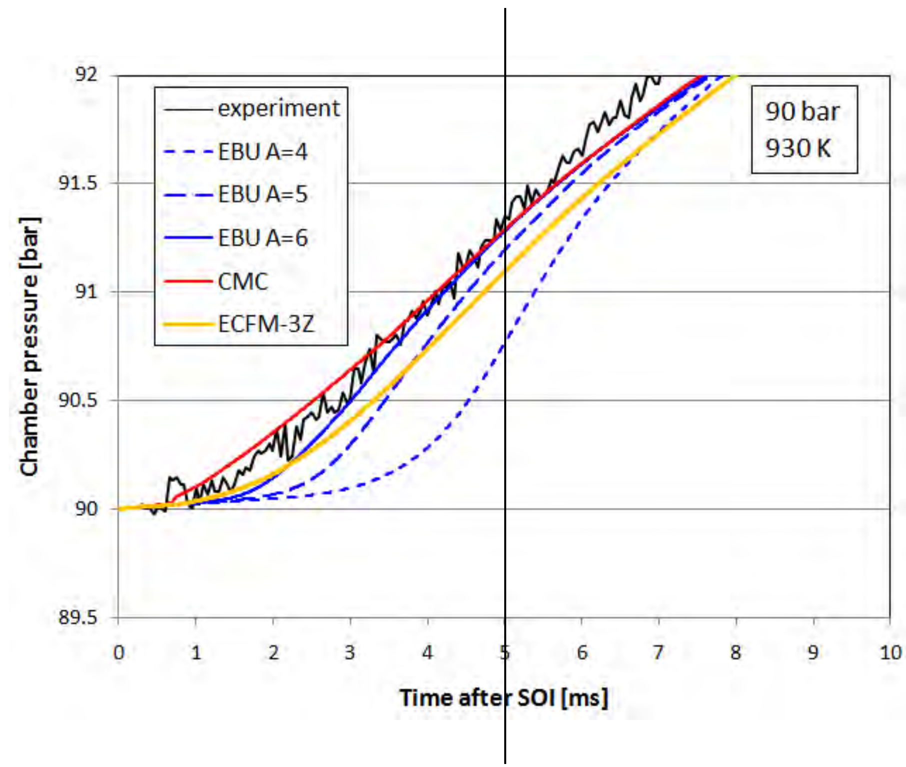
$$- \frac{\nabla \cdot \left(\langle u_i'' T'' | \eta \rangle \langle \rho \rangle \tilde{P}(\eta) \right)}{\langle \rho \rangle \tilde{P}(\eta)} + \underbrace{\frac{1}{\langle c_p | \eta \rangle} \left\langle \frac{1}{\rho} \frac{\partial P}{\partial t} \middle| \eta \right\rangle}_{\text{Time-varying pressure}} + \frac{\langle w_H | \eta \rangle}{\langle \rho | \eta \rangle \langle c_p | \eta \rangle} + \underbrace{\frac{\langle w_{WALL} | \eta \rangle}{\langle \rho | \eta \rangle \langle c_p | \eta \rangle}}_{\text{Wall heat transfer}}$$

Source: De Paola, Mastorakos, Wright & Boulouchos, Combustion Science and Technology 180 (2008)

Pressure trace: Comparison CMC, EBU LaTCT and ECFM-3Z



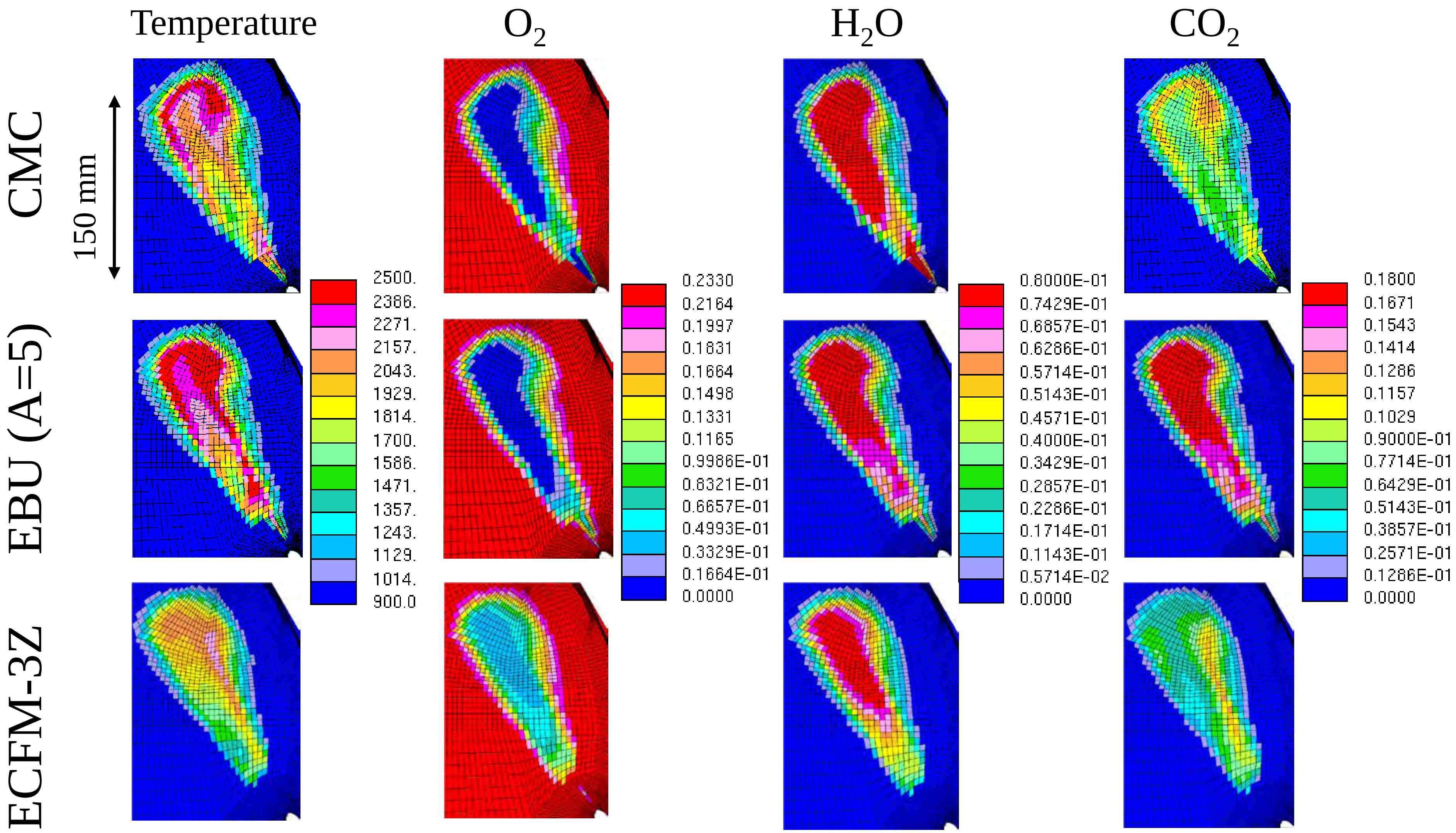
Total injection duration: ~25 ms



- CMC pressure agrees well with EBU and ECFM-3Z in the late phase
- CMC ignition delay well captured
- Discrepancies for all models between 10 and 20 ms

→ Fuel injection rate need needs further investigation (estimate)

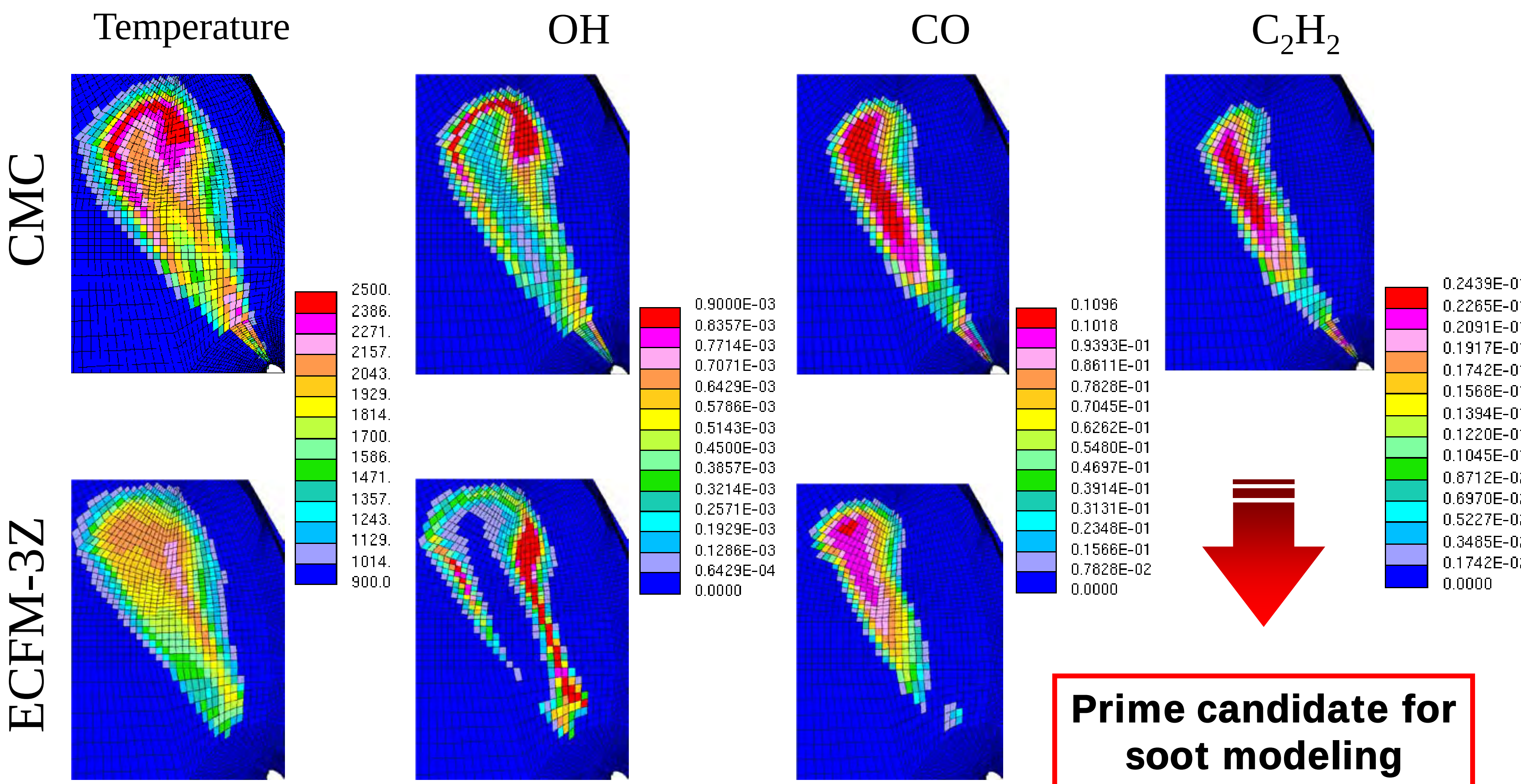
Comparison of major species distributions 5 ms after SOI



ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

WÄRTSILÄ

Comparison of minor species distributions 5 ms after SOI



Prime candidate for soot modeling (precursor)

Conclusions

- **Three combustion models assessed for large marine Diesel engine reference experiment:**
    - Eddy break-up (LaTCT)
    - ECFM-3Z
    - Conditional Moment Closure
- **Differences can be observed w.r.t. ignition phase**
- **Later stage pressure evolutions agree well for all three models**
- **Reasonable agreement for major and minor species distribution for different models (but no validation data available)**

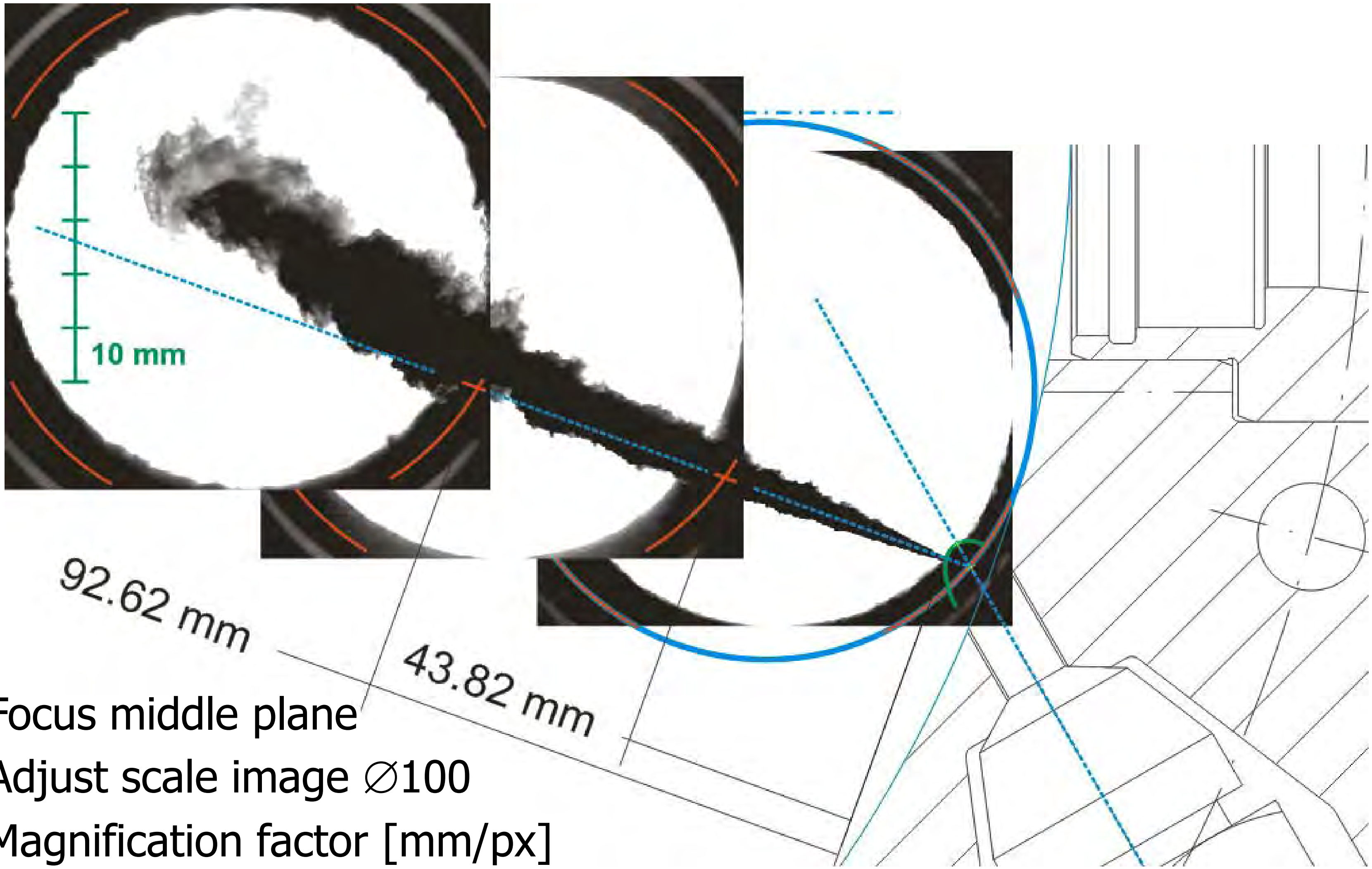
Outlook

- **Modelling:**
  - Compare heat release rates
  - Investigate ignition timing and location, influence of mechanism used*
  - Emissions: NO_x a 'by-product' and soot (needs substantial work)

- **Experiment:**
  - Non-reactive (N_2) for spray plume and dense core discrimination
  - Different fuels: Dodecane, heavy fuel oil
  - Photomultiplier for better ignition detection
  - Chemiluminescence and multi-colour pyrometry data acquisition
  - Droplet size and velocity measurements
  - Heat release calculation from pressure trace
  - How to quantify NO_x?

* cf. Wright, Margari, de Paola, Mastorakos and Boulouchos, Flow, Turbulence and Combustion 84 (2010)

non-reactive (N_2) extended measurement domain

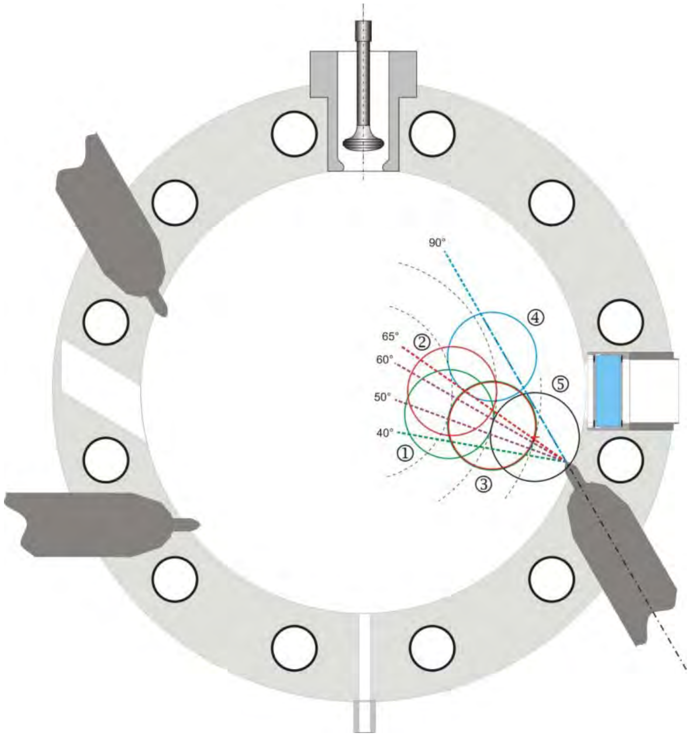


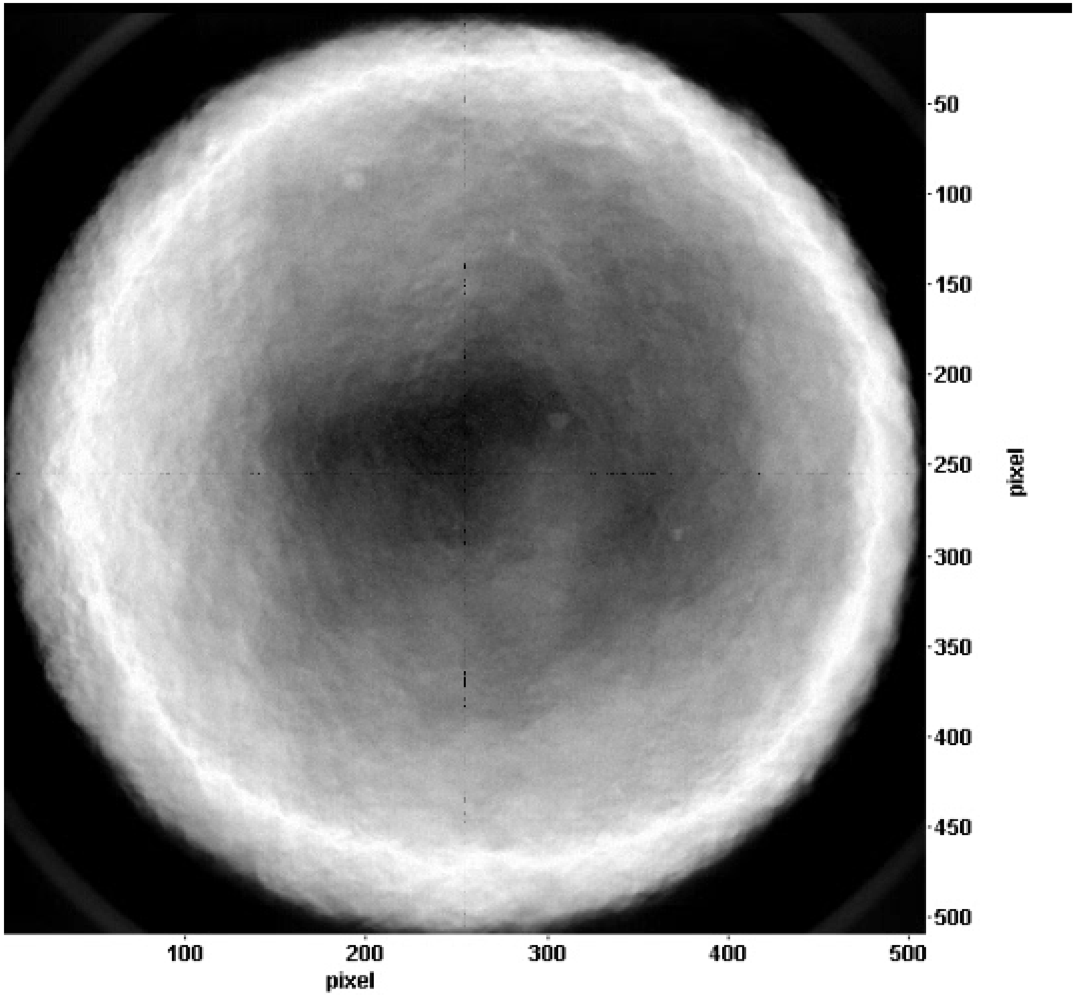
- Focus middle plane
- Adjust scale image ∅100
- Magnification factor [mm/px]
- Define origin nozzle exit

Source: Herrmann, von Rotz, Schulz, Weisser, Boulouchos, Schneider, ILASS 2010

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Discriminate between dense core and spray plume penetration





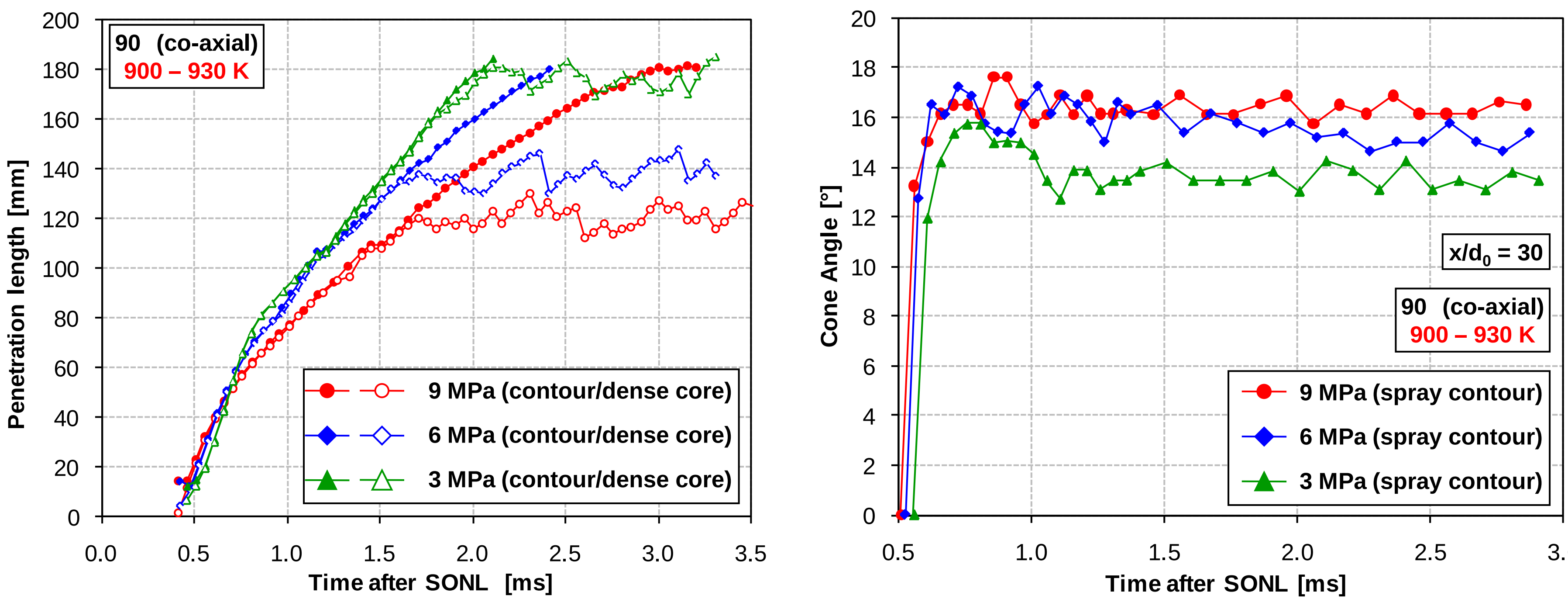
Source: Herrmann, von Rotz, Schulz, Weisser, Boulouchos, Schneider, ILASS 2010

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

WÄRTSILÄ

Spray penetration length and total cone angle

variation of chamber pressure



- Spray propagation: linearly (first stage), afterwards with ~$t^{0.5}$
- Spray contour and dense core separation
- Dense core stabilization (fluctuation)
- Additional effects (swirl influence)

Source: Herrmann, von Rotz, Schulz, Weisser, Boulouchos, Schneider, ILASS 2010

Acknowledgements / funding / collaborations

- EU Projects HERCULES (FP6) and HERCULES-Beta (FP7)
- Swiss Federal Office of Energy (BfE) – Dres. Hermle & Renz
- Paul Scherrer Institute, Switzerland
- University of Cambridge – Prof. E. Mastorakos et al.
- cd-adapco development and support

Eidgenössische Technische Hochschule Zürich
Ecole polytechnique fédérale de Zurich
Politecnico federale di Zurigo

Thank you

32nd IEA Task Leader Meeting, Nara, Japan, Jul. 2010

Michele Bolla[*], Yuri M. Wright[*,†] and Konstantinos Boulouchos[*],
Kai Herrmann[‡] and Beat von Rotz[‡]

Aerothermochemistry and Combustion Systems Laboratory, ETH Zürich, Switzerland
[‡] Wärtsilä Switzerland, Ltd.

[†] mailto:wright@lav.mavt.ethz.ch