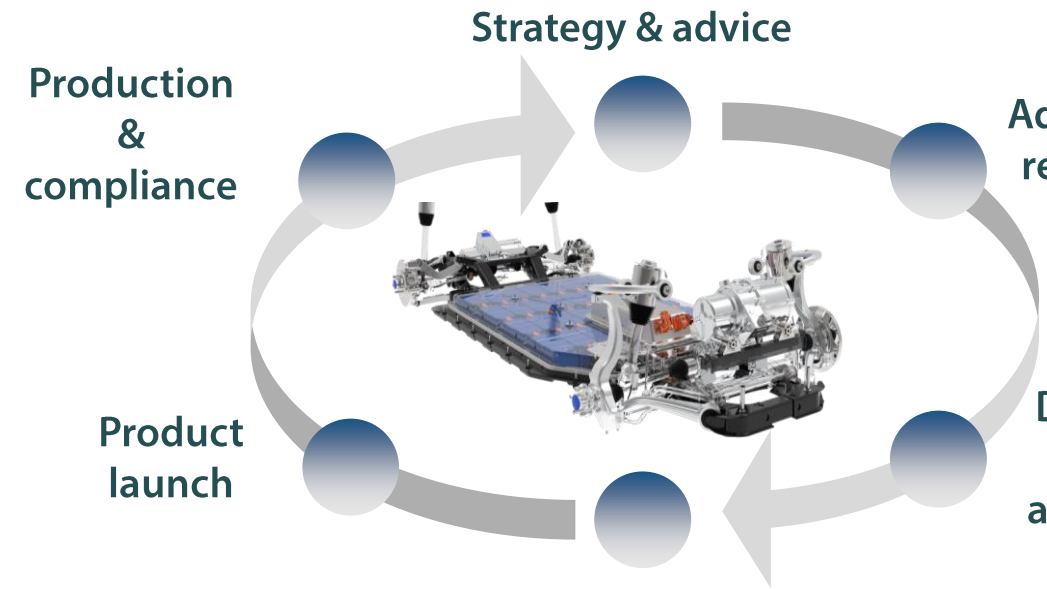
Managing complexity in internal combustion engine modelling for virtual product development

E. Shapiro, C. Turquand D'Auzay, I. Ahmed, I. Hernandez

Ricardo Software

ABOUT RICARDO

Est. 1915
3,000 People
55 Sites
9 Engineering Delivery Centres
21 Countries
£352m Revenue (19/20)



Automotive | Commercial Vehicle | Off-Highway & Industrial | Personal Transport | Aerospace | Defence | Marine | Rail | Energy

Ricardo Software

COMPLEX SYSTEMS

STRUCTURAL MECHANICS

FLUID DYNAMICS

SOFTWARE SOLUTIONS

112+

People & Footprint

Working in 10 locations across 7 countries

100+

Customers

In 15 countries. – key geographies include China, India, Europe and the US

Automotive Solutions

Virtual Calibration

Energy Management

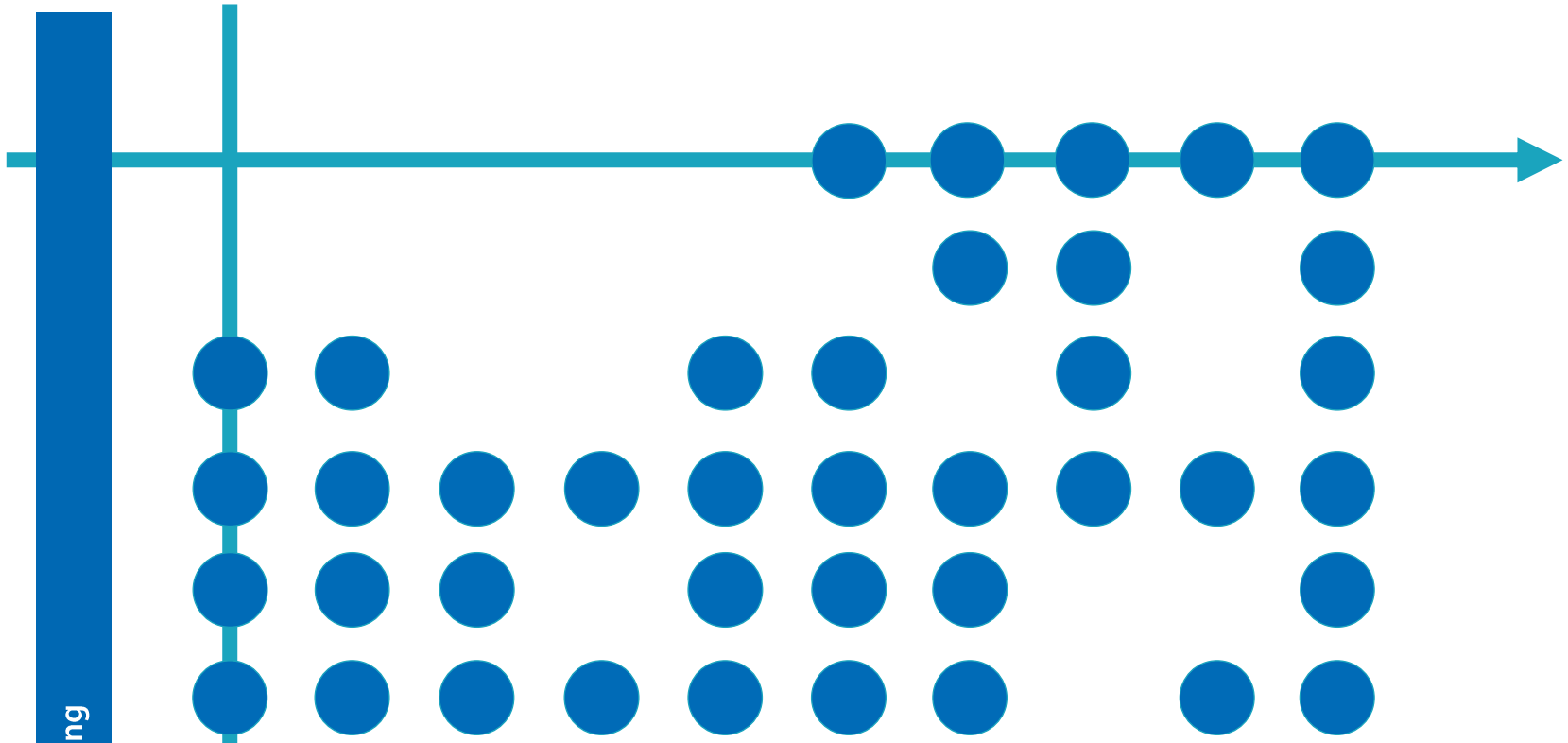
Driveline Dynamics

Electrification

NVH

Durability

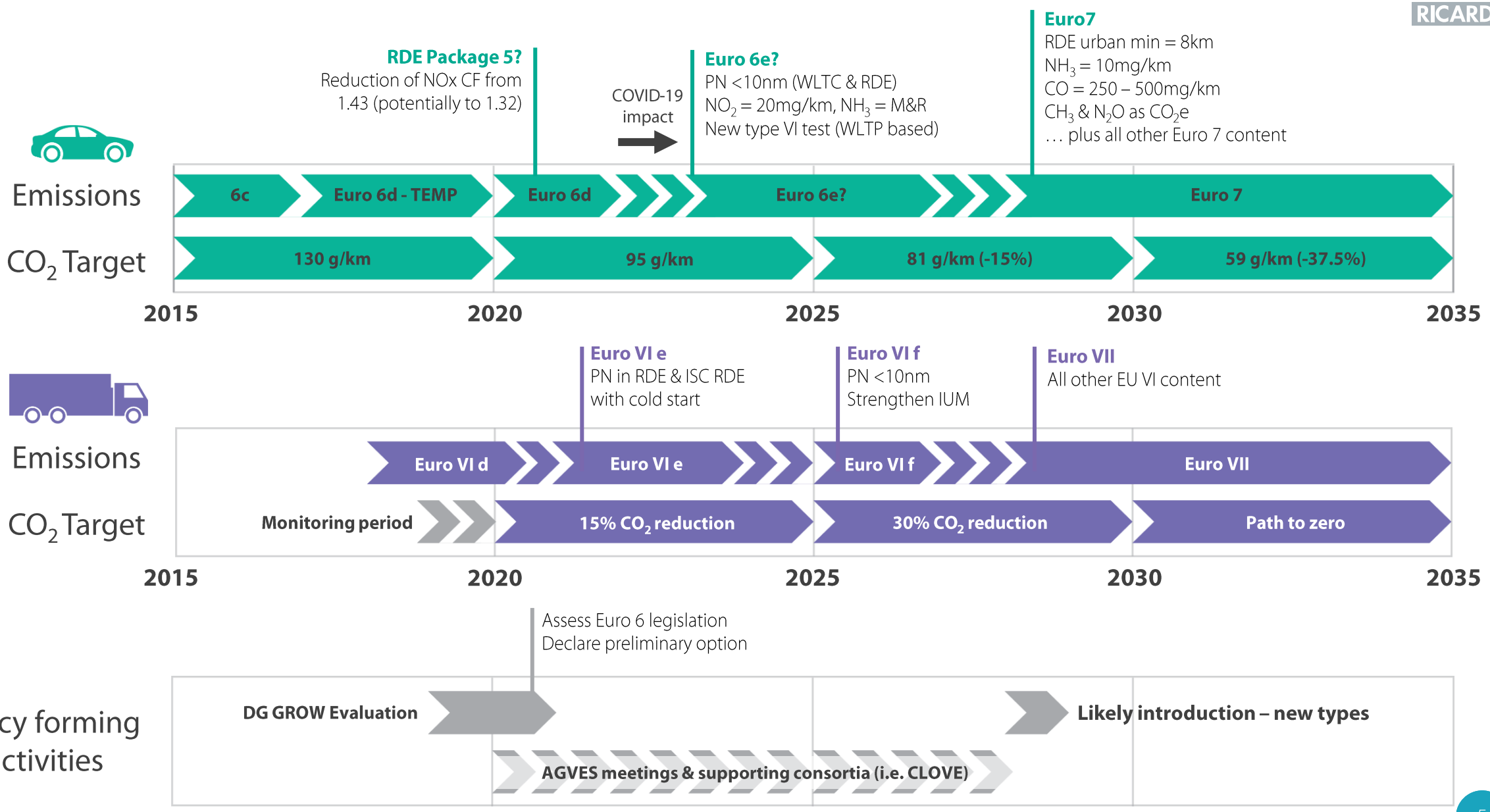
Integration / Sequencing



Continues across all sectors

Key enabler for customers is integration / sequencing and model management

Ricardo's **estimated** timeline for new EU emissions legislation introduction



*The content is a Ricardo view of potential future regulations and solutions and does not reflect the current and on-going discussions within the CLOVE consortium for the development of the post EURO 6 standards.

Renewable chemical fuels for ICEs are an alternative to electrification - The landscape

Crop

Advanced / waste

Biomass

Electricity (Renewable or generated in process)

Water

Carbon dioxide

Bio Energy with Carbon Capture (BECC)

Direct Air Capture (DAC)

Electrolysis

Steam reforming

Synthesis gas

Hydrogen

Broadly mechanical and organic chemistry processes. E.g.
- Pressing / Rendering
- Distillation
- Hydrotreating
- Fermentation
- Digestion
- Esterification

Ethanol | Biodiesel | Hydrogenated Vegetable Oil | Biogas

Biofuels

More intensively chemical processes with catalysis. E.g.
- Fischer-Tropsch
- Methanol synthesis
- OME / DME synthesis

FT liquids | DME / OME | Bio-methanol

Synthetic Biofuels

Hydrogen

Zero TTW Carbon

Ammonia

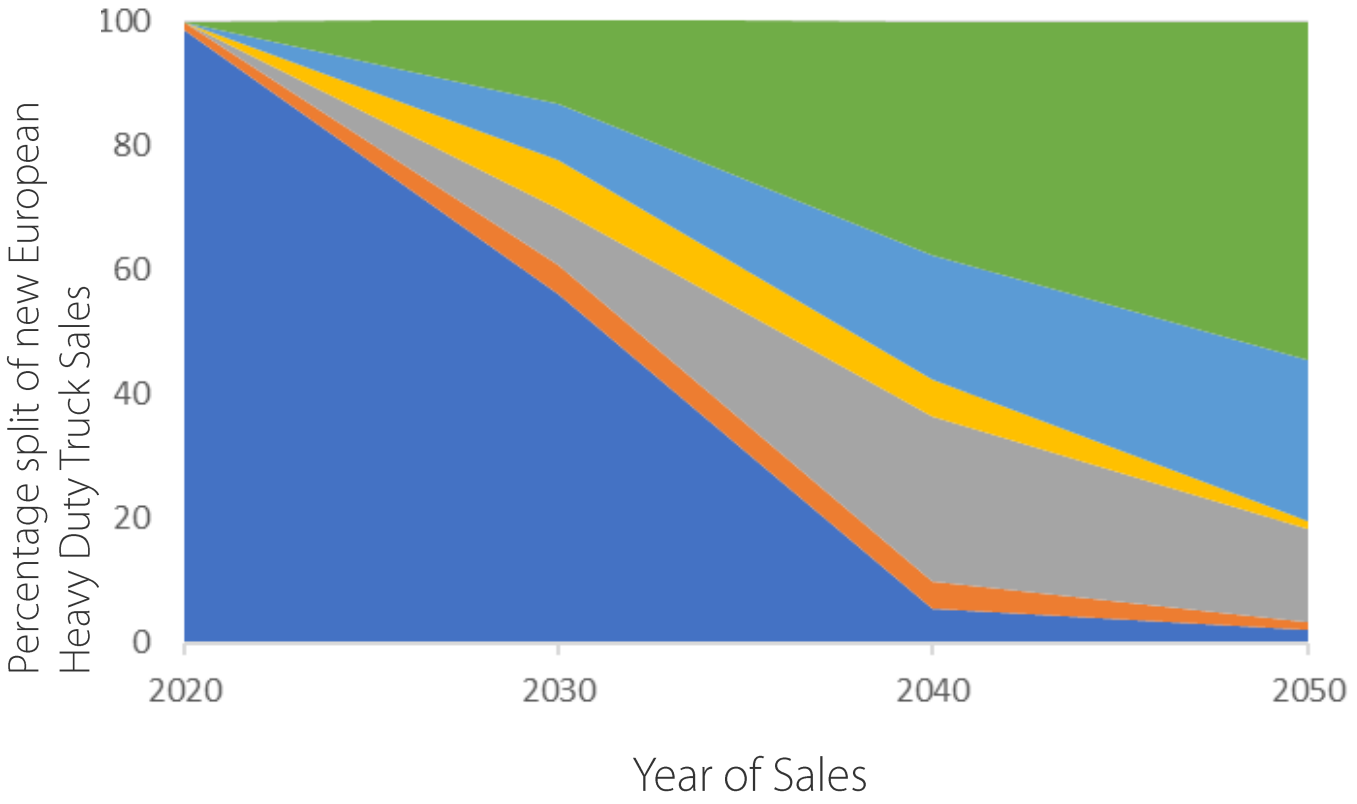
Synthesis e.g.
- Haber-Bosch (ammonia)
- RWGS + Fischer-Tropsch
- Methanol dehydration
- Sabatier (methane)
- Methanol synthesis

Methane | F-T HCs | Methanol | D / OME

E-fuels

European OEMs are projecting phase out of diesel products by 2040
By 2035 zero carbon propulsion will dominate including Battery, Fuel Cell and H2 ICE

Ricardo Projection of European Long Haul Truck Sales by Propulsion System



- Conventional Diesel ICE
- CNG/LPG
- Renewable fuelled ICE
- Hybrid ICE
- Battery including ERS
- Fuel Cell

Challenges of Euro VII and CO2 legislation. Majority of European OEMs have announced phase out of diesel combustion engines by 2040.

CNG and LPG have small current market penetration. They are not zero carbon, and have future emissions challenges. Unlikely to experience large uptake.

Depending on regulatory rules, renewable fuels could be large part of future propulsion. Long term this is likely to be zero carbon fuels such as H2

Maybe introduced short term to support last mile deliveries in geofenced areas, but limited volume

Challenges from payload reduction, battery size, and charging infrastructure, but could be used on shorter distances or controlled routes

Offers better Total Cost of Ownership than Battery only solutions together with range benefits. Take up dependant on infrastructure and cost reduction.

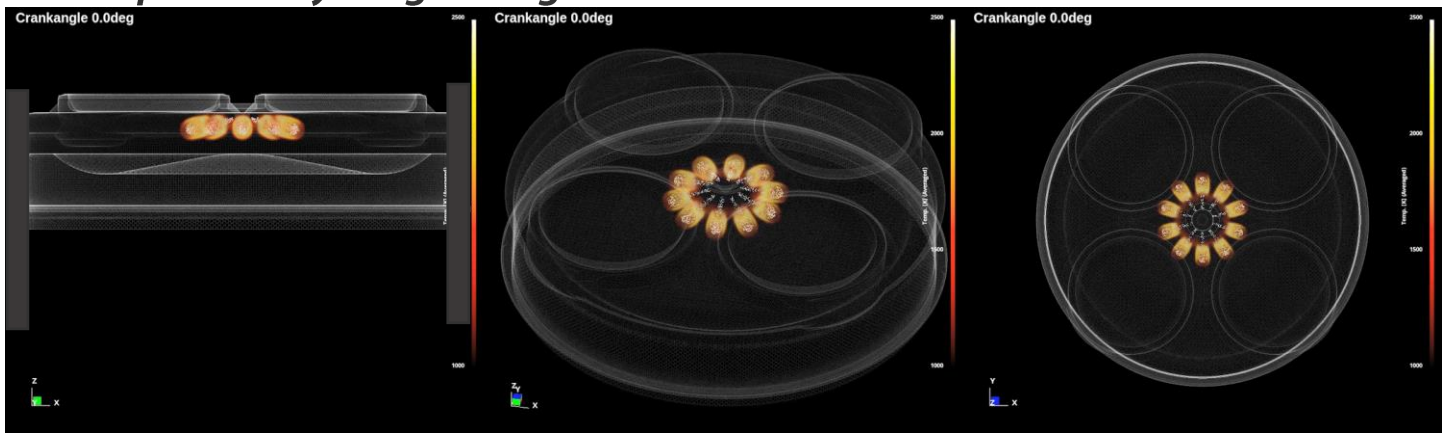
Predictive Modelling

- Predictive 3D combustion modelling
- Predictive 3D emissions modelling
- Predictive 3D thermal modelling
- Simulation timescales compatible with Virtual Product Development. Approximate maximum constraints: 2 days/cycle, 128 cores/2-3m cells ~ **6k core-hours/cycle**

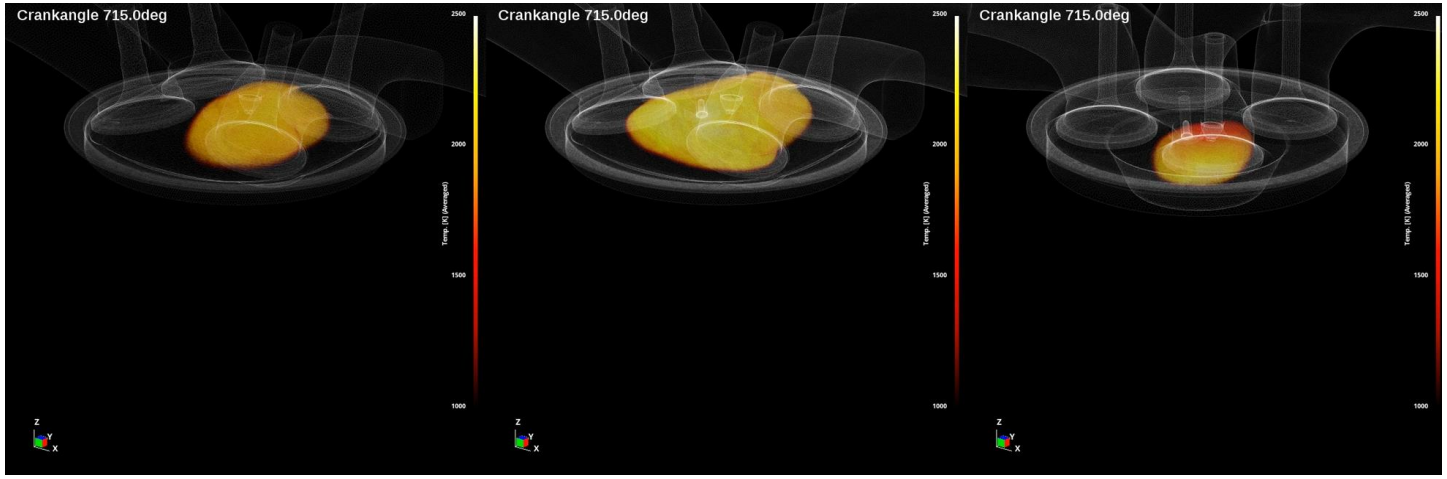
Complexity in 3D CFD ICE Modelling

- Motion model
- Spark model
- Kinetics model
- Grid resolution
- Wall boundary conditions
- Turbulence model
- I/O boundary conditions
- Combustion models
- Spray model
- Initial conditions
- Wall film model
- Emissions models

Diesel piloted hydrogen engine combustion



Hydrogen engine bowl design



Challenge: Motion Modelling

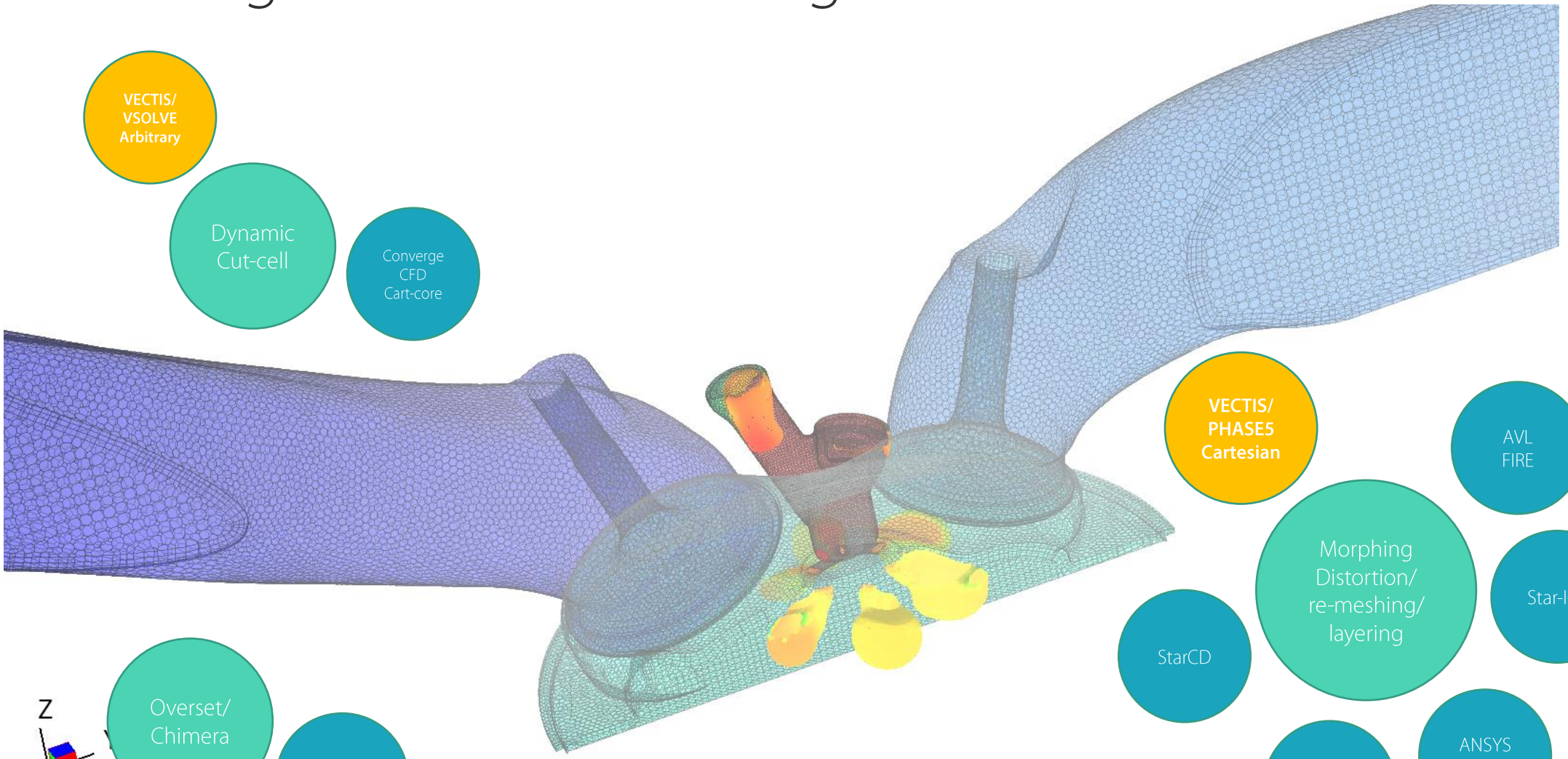
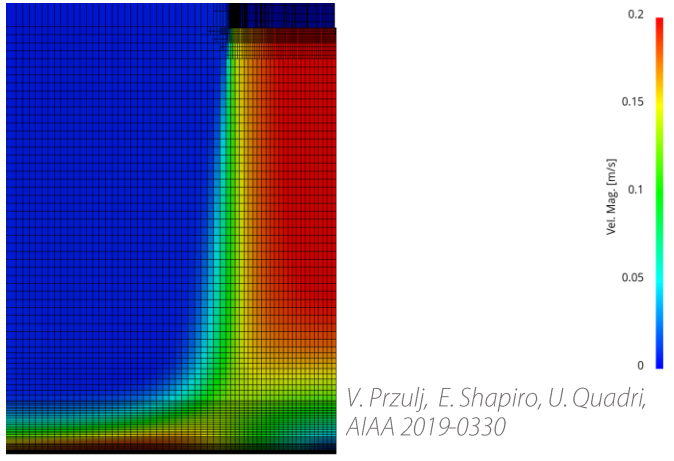


Image: Magma xEV/PC version VECTIS/VSOLVE.
Also see: https://www.youtube.com/watch?v=rqoJr_VoSV8

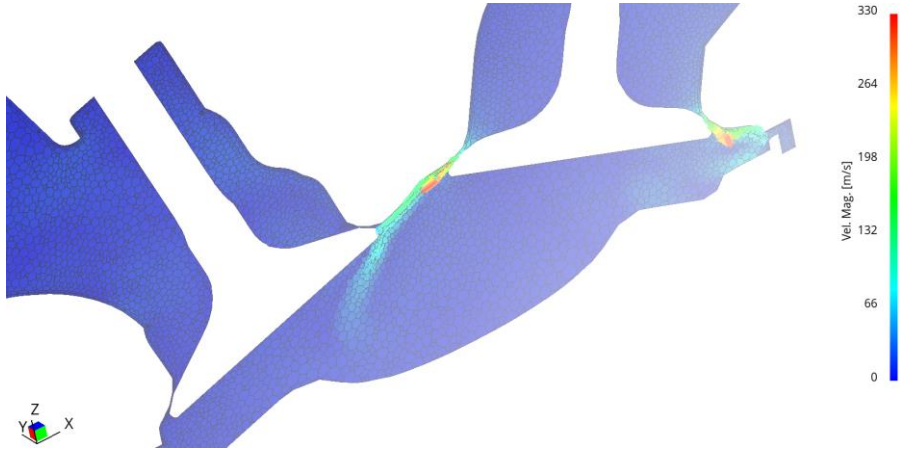
Challenge: Grid Resolution

Impinging Jet Flow, incompressible, Re~70,000: **~50 cells across the jet**

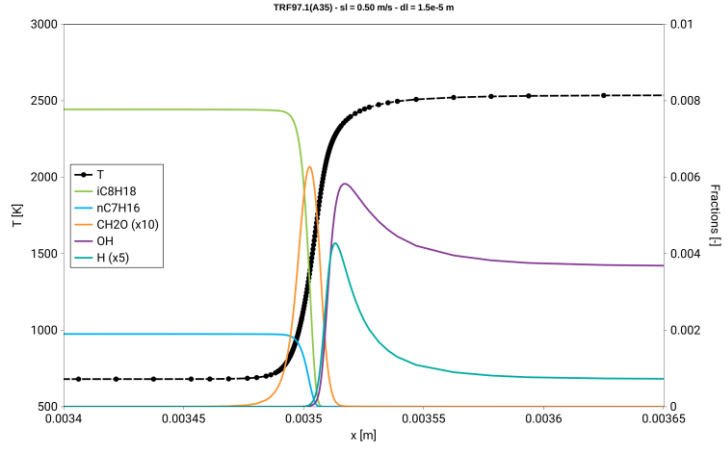


V. Przulj, E. Shapiro, U. Quadri, AIAA 2019-0330

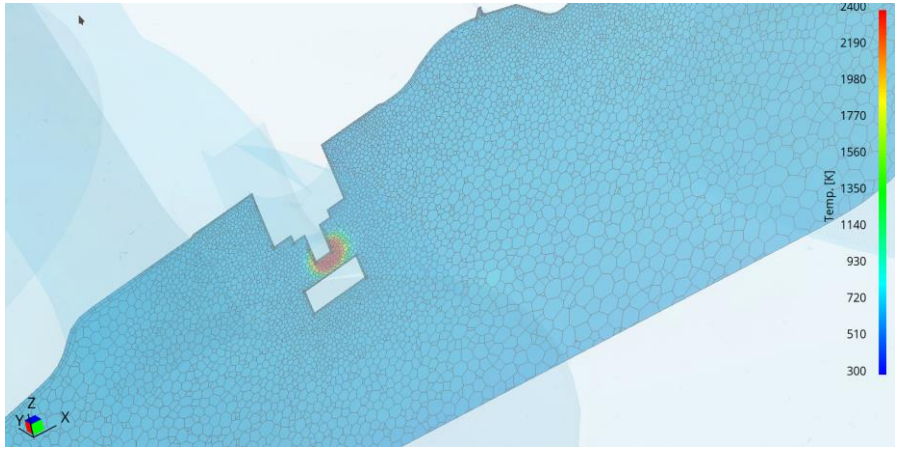
GDI, IVO, Ma~0.9, Re~80,000 (2mm): **5 cells across the jet**



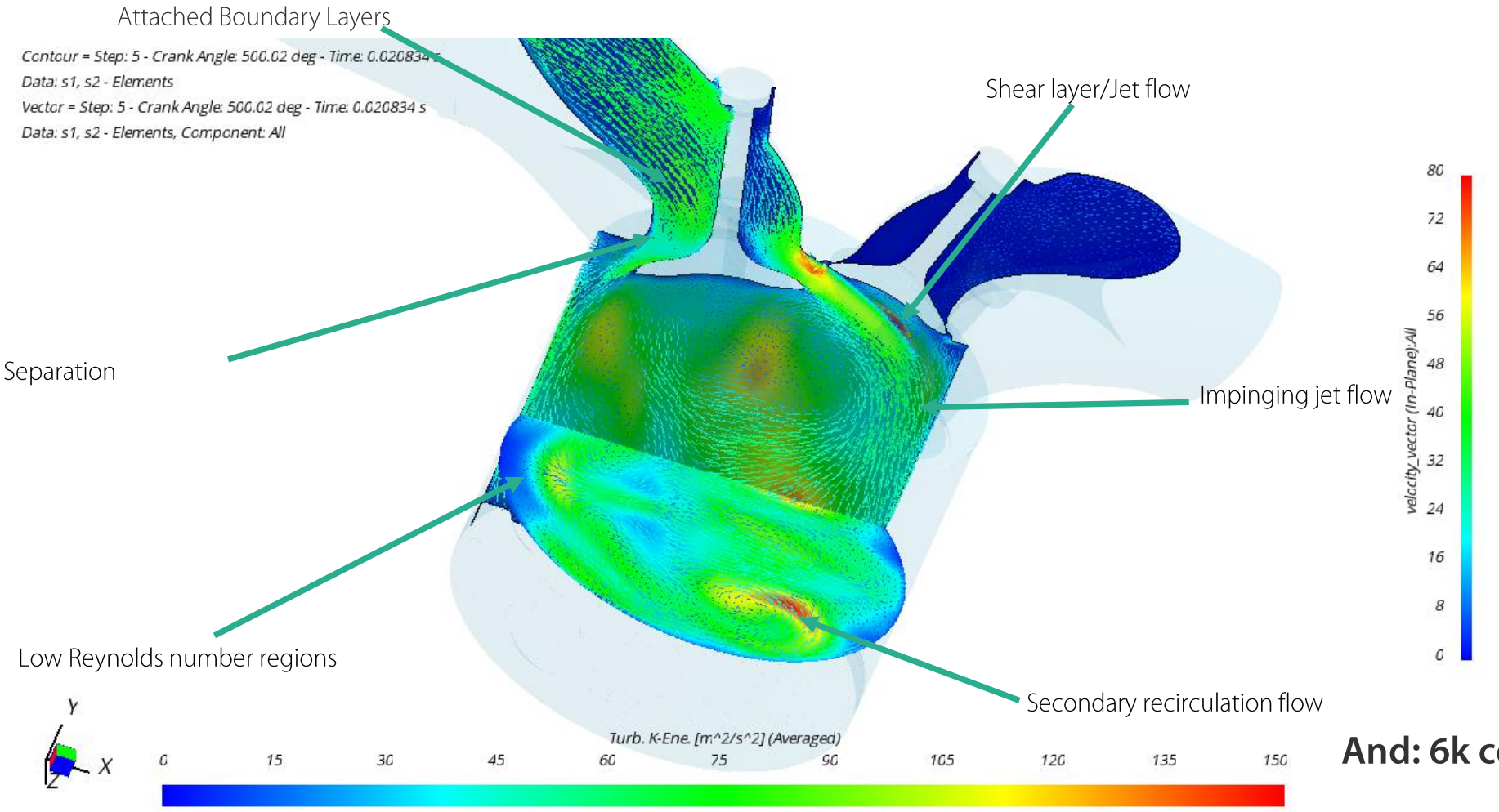
Typical direct calculation with Ricardo Combustion Toolbox, P=45bar, T=680K, Sl=0.5m/s, δl~0.02mm
SIP TRF 97.1RON, **Symbols represent grid points.**



GDI, Spark time – Sl~0.75m/s, T=680K, P=45bar, δl by χ/Sl= 0.0035mm
Li~0.1-3mm, Cell size - 0.1-0.2mm kernel, 0.4-0.5mm core



Challenge: Turbulence model

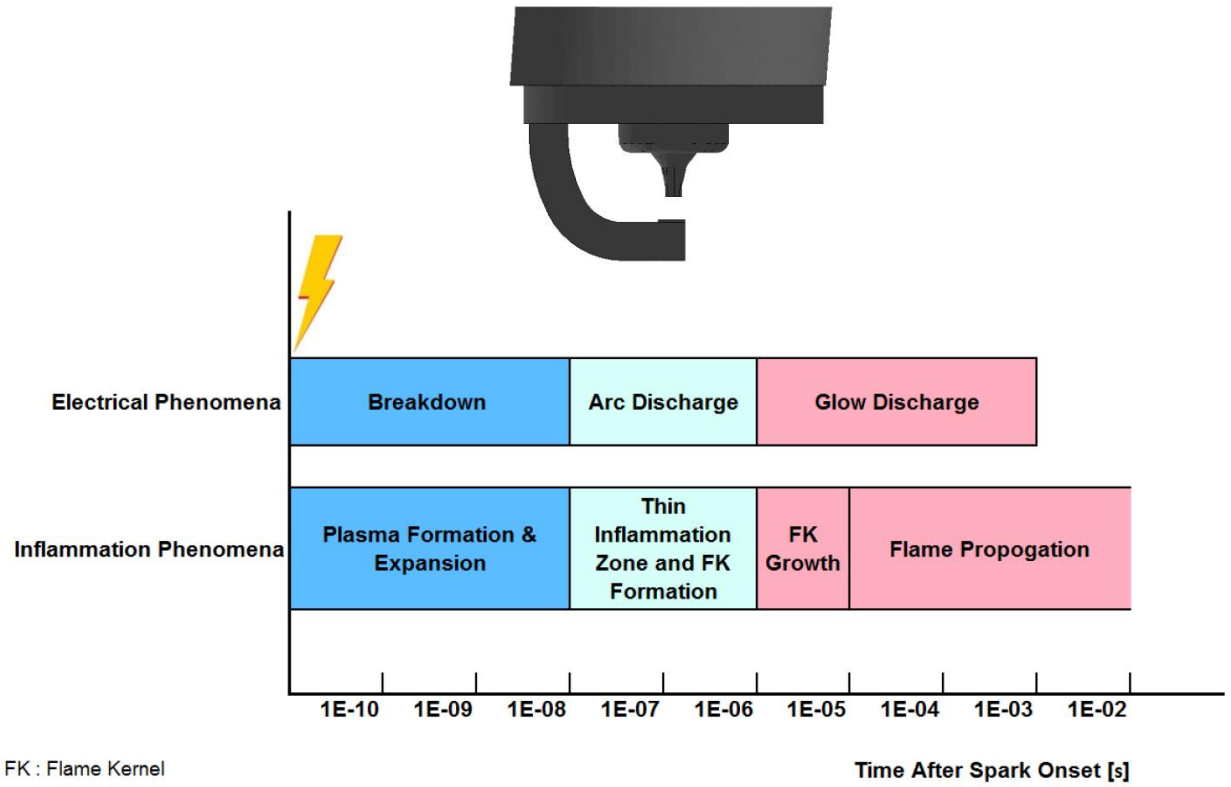


Requirements:

- ✓ Consistent and accurate resolution of both free-shear and wall turbulence
- ✓ Accurate heat transfer prediction
- ✓ Accurate prediction of integral length scale and turbulence properties required for the combustion closures: **Flame Speed**

And: 6k core-hours/cycle

Challenge: Spark modelling



G. Tallu, L. M. Beck, M. Prouvier, A. Winkler, M. Frambourg, E. Shapiro, "3D CFD Modelling and Simulation of Spark Ignition inclusive Turbulence Effects and Detailed Chemical Kinetics, IAV 2016,

Requirements:

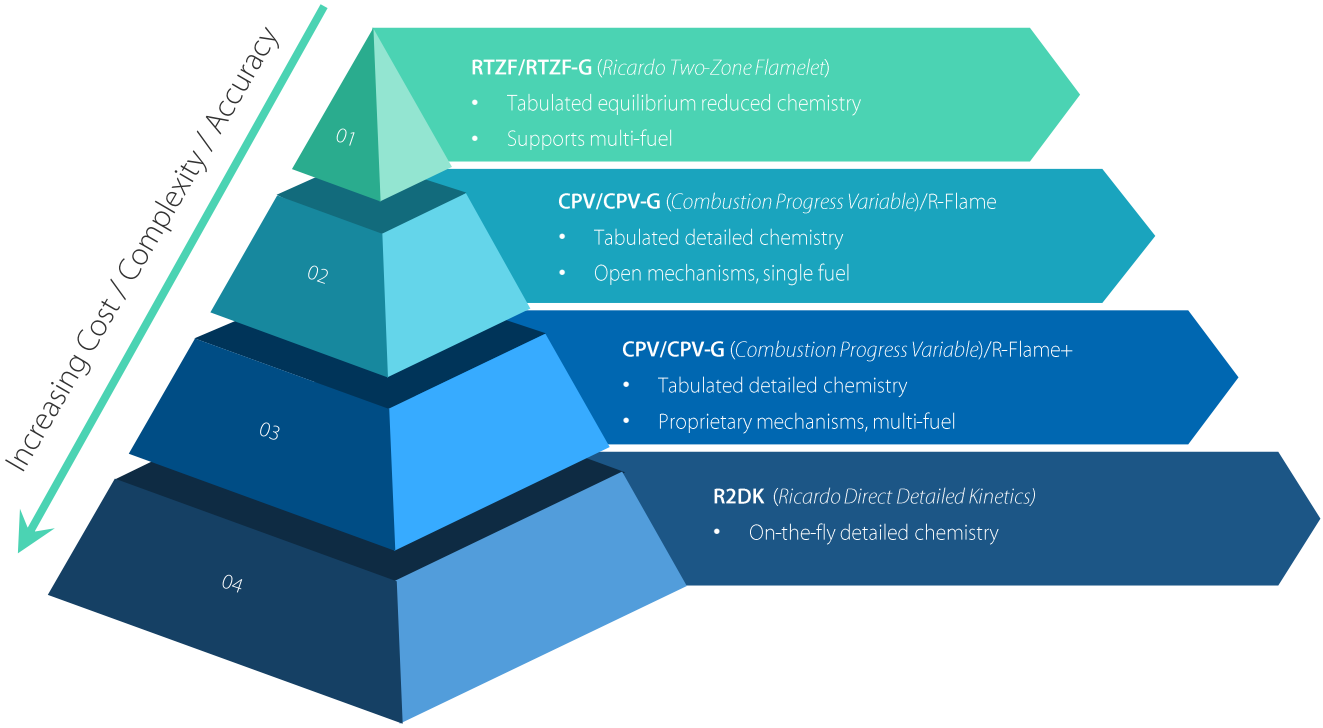
- ✓ Accurate geometry resolution at scales of spark plug gap
- ✓ Accurate modelling of heat losses
- ✓ Resolution of the initial flame kernel size and position
- ✓ Resolution of initial stages of hot kernel development at T~10-60,000K
- ✓ Resolution of arc and glow stages of discharge
- ✓ Composition/chemistry misfire modelling
- ✓ Turbulence induced misfire modelling

And: 6k core-hours/cycle

Challenge: Combustion modelling

Requirements:

- ✓ Multiple fuels support (e.g. H2/CH4, Diesel/H2, Diesel/CH4)
- ✓ Multi-component fuels support (e.g. gasoline ETRF blends)
- ✓ Premixed/non-premixed agnostic (semi-premixed)
- ✓ Accurate thermochemistry (power output)
- ✓ Sufficient data for emissions modelling
- ✓ Flame-wall interaction and crevice quenching resolution



And: 6k core-hours/cycle

Calibrated Modelling

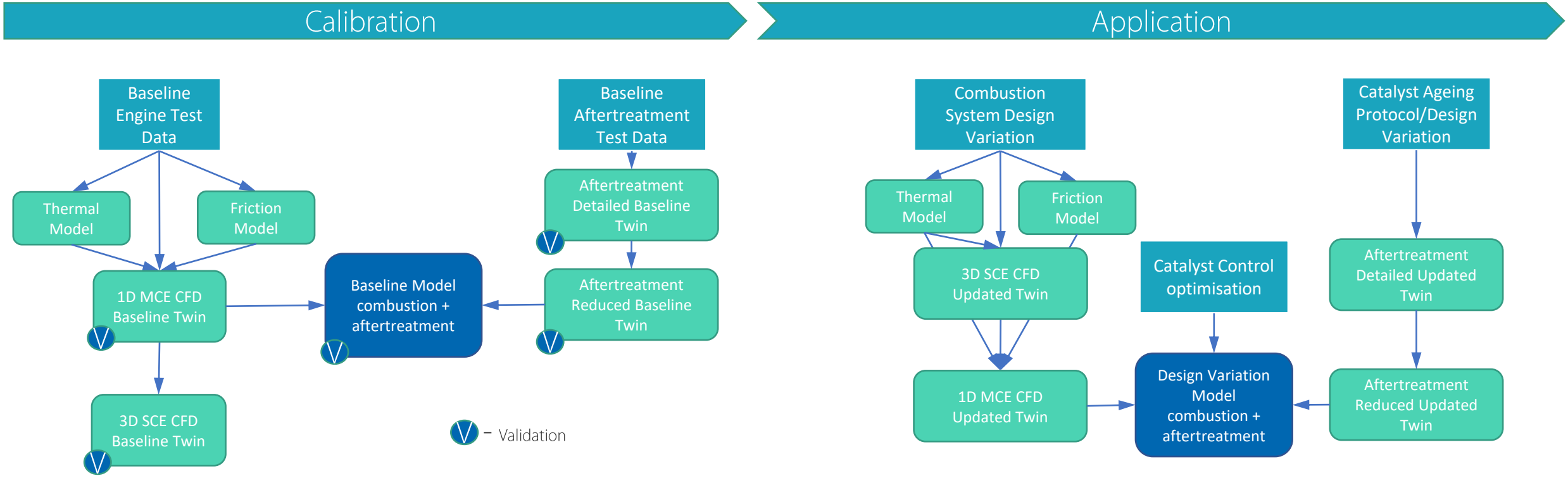
Calibrated 3D combustion modelling

Calibrated 3D emissions modelling

Calibrated 3D thermal modelling

Simulation timescales compatible with Virtual Product Development

Calibration/Application Workflow



Calibrate once for a baseline, apply for all parametric variations

- ✓ Run-times constraints: 6k core-hours/cycle
- ✓ Number of simulations required ~100-200

Case study: CNG PCI Development

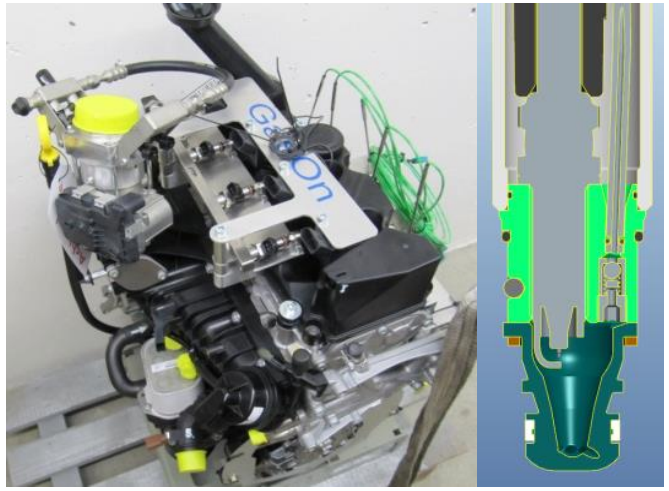
- ✓ λ=1.4-1.7 with brake engine efficiency up to 45% at 1.7.
- ✓ Stable ignition is possible up to λ=2.2
- ✓ Can operate without scavenging up to λ=1.6

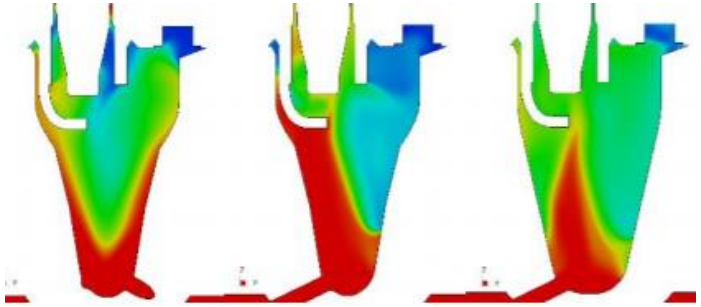
VOLKSWAGEN AKTIENGESELLSCHAFT

- ✓ Hardware development and integration (including CAE)
- ✓ Coordination of work

Ricardo Software
Powertrain CAE Solutions

- ✓ CFD models development and integration in VECTIS suite
- ✓ CFD analysis providing guidance to hardware development





LAV Empa Materials Science and Technology

IDSC

- ✓ LES-CFD analysis, flow physics fundamentals
- ✓ Fundamental experimental campaign
- ✓ Full engine control strategy
- ✓ Full engine testing

Politechnika Poznańska – Poznan University of Technology

- ✓ Single cylinder engine testing and benchmarking
- ✓ Fundamental experiments

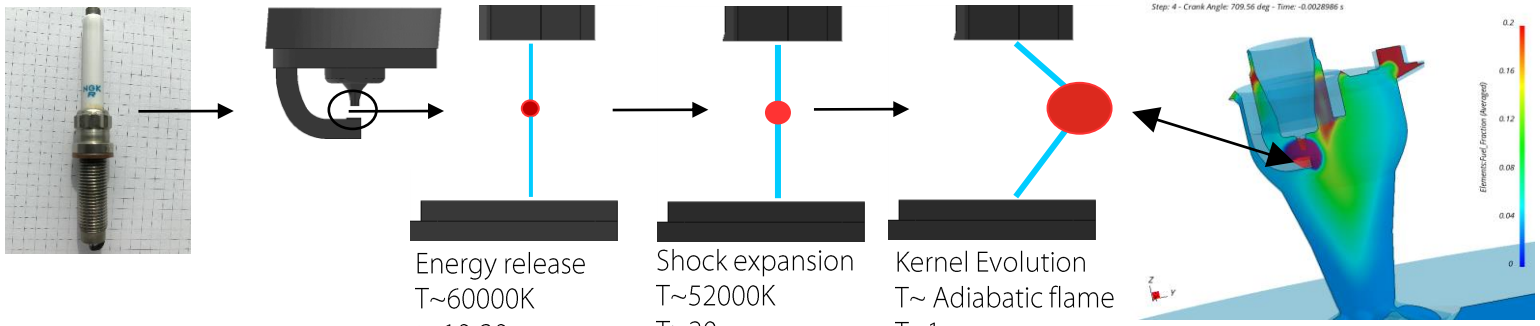
Continental

- ✓ On-board gas quality sensor development and integration

http://gason.eu/

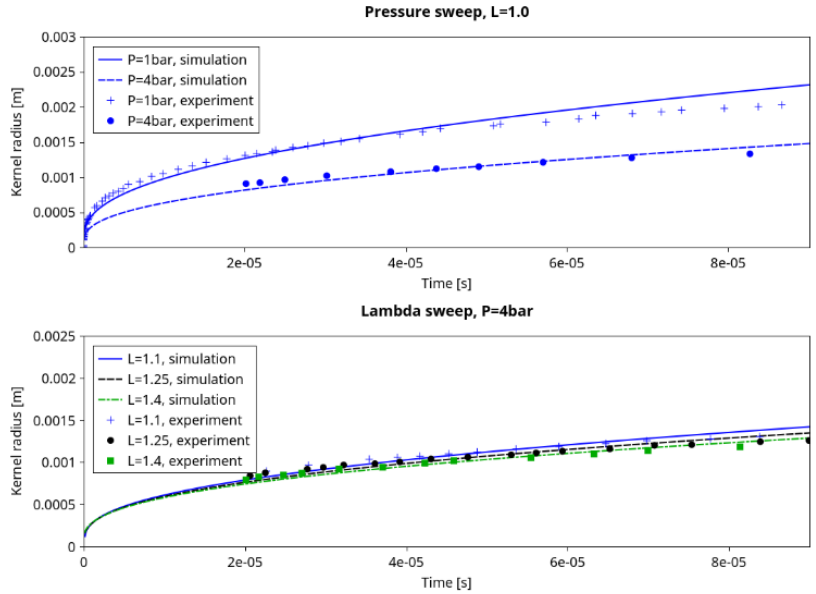
Case study: CNG PCI Development

Test | **0D Modelling** | **3D Modelling**



$$\begin{cases} \frac{dr_k}{dt} = \underbrace{\frac{R_k T_k}{R_u T_u} S_b}_{\text{source (flame)}} + \underbrace{\frac{r_k}{3} \frac{1}{R_k T_k} \frac{d(R_k T_k)}{dt}}_{\text{source (expansion)}} - \underbrace{\frac{r_k}{3} \frac{1}{P_u} \frac{dP_u}{dt}}_{\text{source (external compression)}} \\ \frac{dT_k}{dt} = \underbrace{\frac{W}{\frac{4}{3}\pi r_k^3 \rho_u} \frac{\gamma_k - 1}{\gamma_k} \frac{T_k}{R_u T_u}}_{\text{source (plasma)}} + \frac{3}{c_{p,k} r_k} \left(LHV_{mix} - \left(c_{p,k} \left(T_k - T_0^{std} \right) - c_{p,u} \left(T_u - T_0^{std} \right) \right) \right) \underbrace{\frac{R_k T_k}{R_u T_u} S_b}_{\text{sink (expansion)}} + \underbrace{\frac{\gamma_k - 1}{\gamma_k} \frac{T_k}{P_u} \frac{dP_u}{dt}}_{\text{source (external compression)}} \end{cases}$$

Maly & Vogel benchmark experiment (Proc. Comb. Institute, 1978).

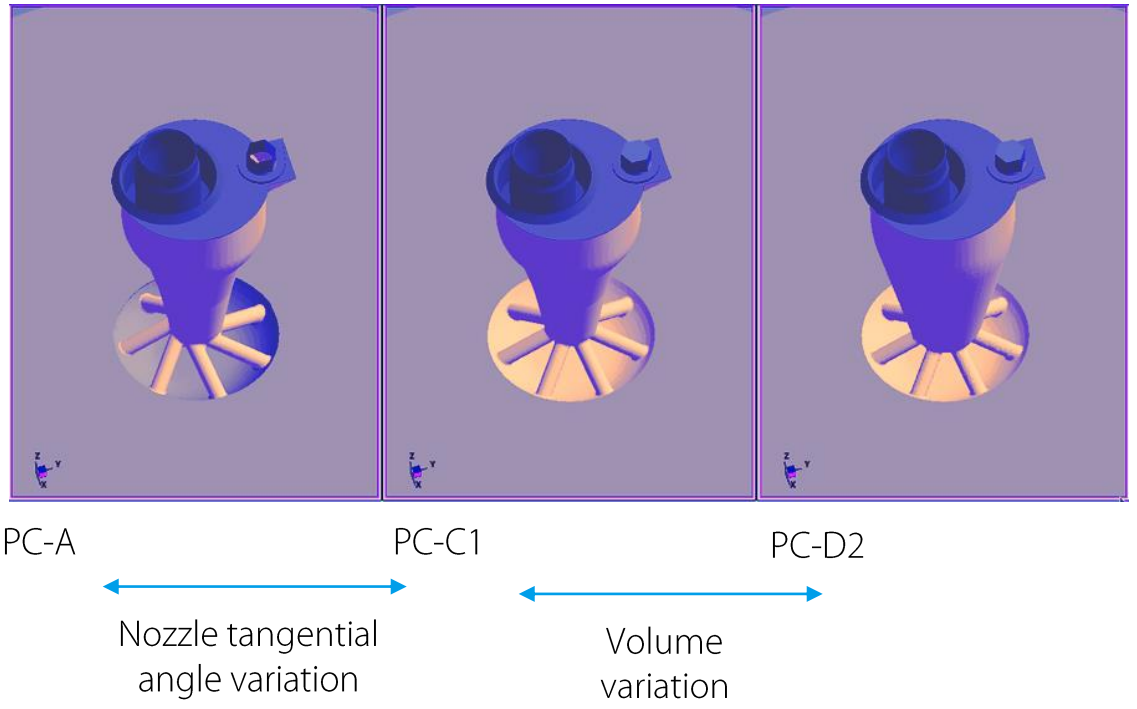


- ✓ Mass and energy conservation resolved directly.
- ✓ Coupling with 3D through front-averaging.
- ✓ Further validation in an optically accessible engine for SI NG set-up (Tallu et al, IAV2016)

Case study: CNG PCI Modelling

PCI configurations:

- ✓ Initial pre-chamber – optimisation from a baseline design existing within Volkswagen Audi Group based on the mixture homogeneity target
- ✓ Within the project, volume, nozzle configuration and orientation were the primary design vectors
- ✓ RCEM comparison with equivalent rpm of 600
- ✓ Pure methane

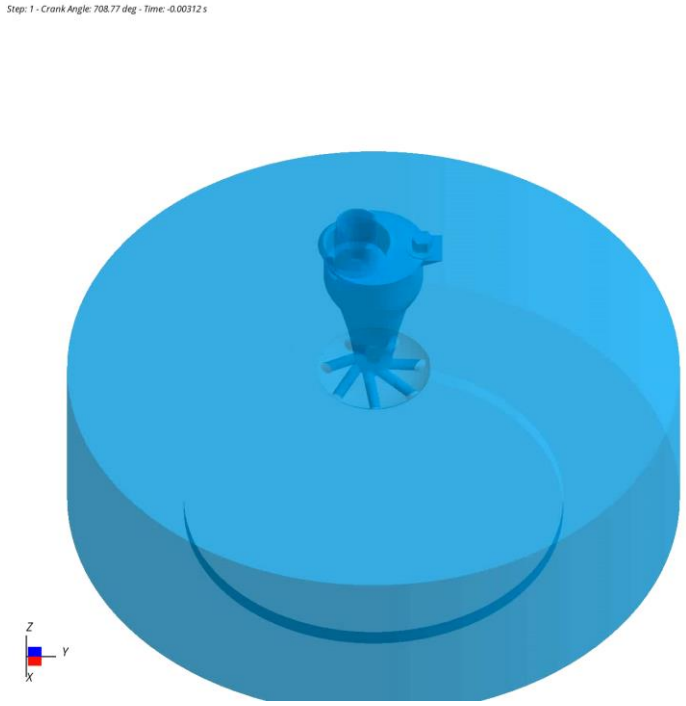


Shapiro, E., Tiney, N., Kyrtatos, P., Kotzagianni, M. et al., "Experimental and Numerical Analysis of Pre-Chamber Combustion Systems for Lean Burn Gas Engines," SAE Technical Paper 2019-01-0260, 2019, doi:10.4271/2019-01-0260.

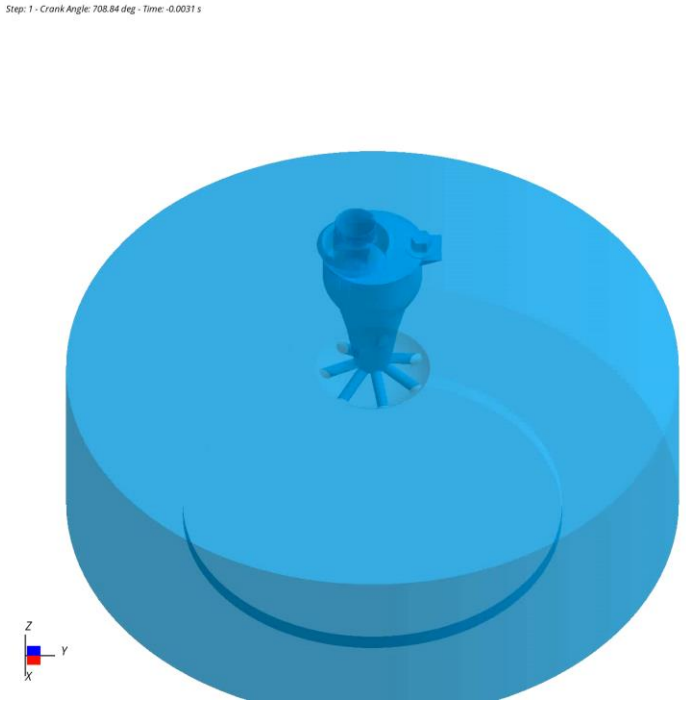
Case study: CNG PCI Development

Spark: DDPIK model, **Combustion:** RTZF/G/G-variance, **Thermochemistry:** 0D equilibrium, **Turbulence:** k-e Time Scales Bounded

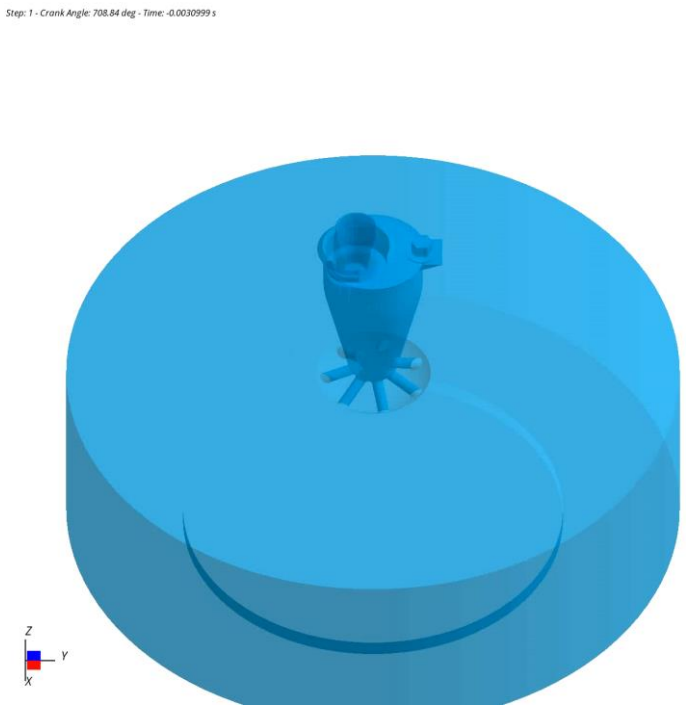
PC-A



PC-C1



PC-D2

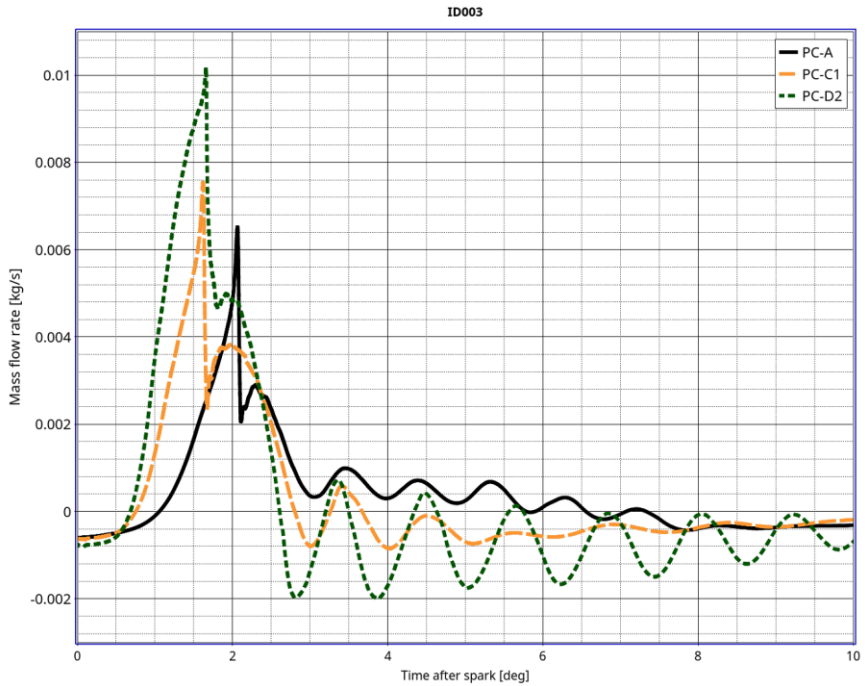


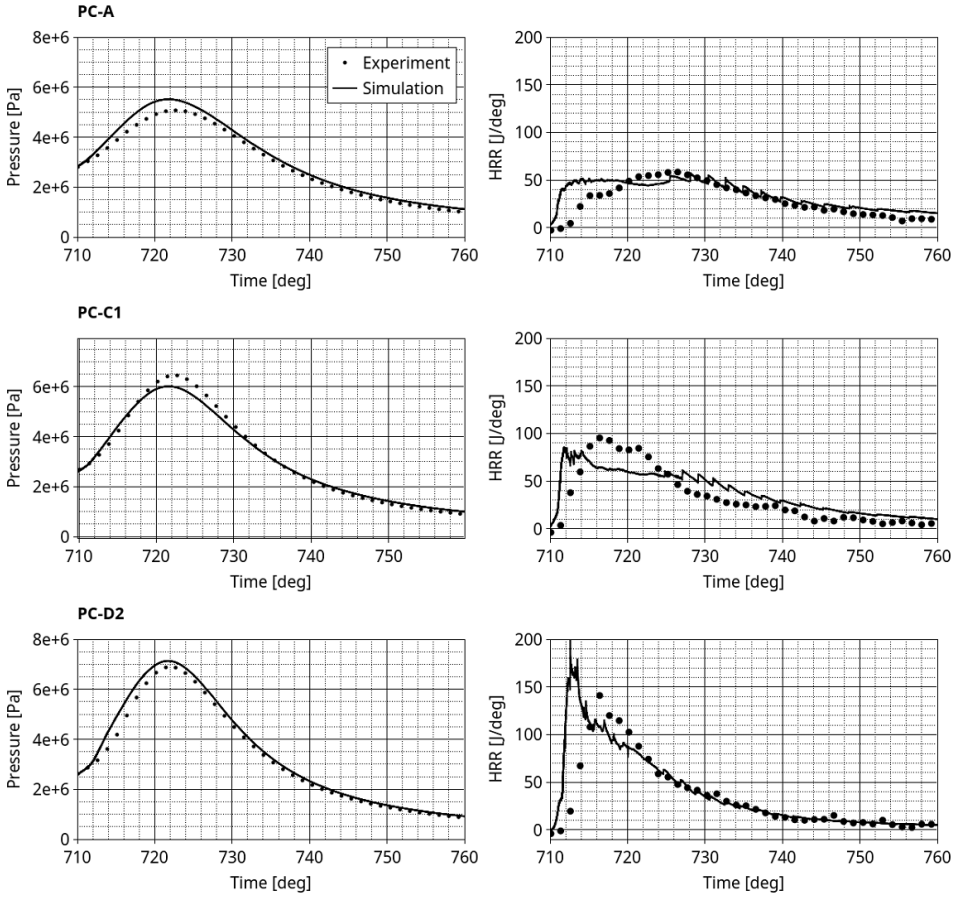
Shapiro, E., Tiney, N., Kyrtatos, P., Kotzagianni, M. et al., "Experimental and Numerical Analysis of Pre-Chamber Combustion Systems for Lean Burn Gas Engines," SAE Technical Paper 2019-01-0260, 2019, doi:10.4271/2019-01-0260.

http://gason.eu/

Case study: CNG PCI Development

- Good agreement with the experimental data with the same CFD tuning point for all pre-chambers and all lambdas
- As in the experiment, pre-chamber PC-D2 delivers faster heat release through more powerful flame jets:



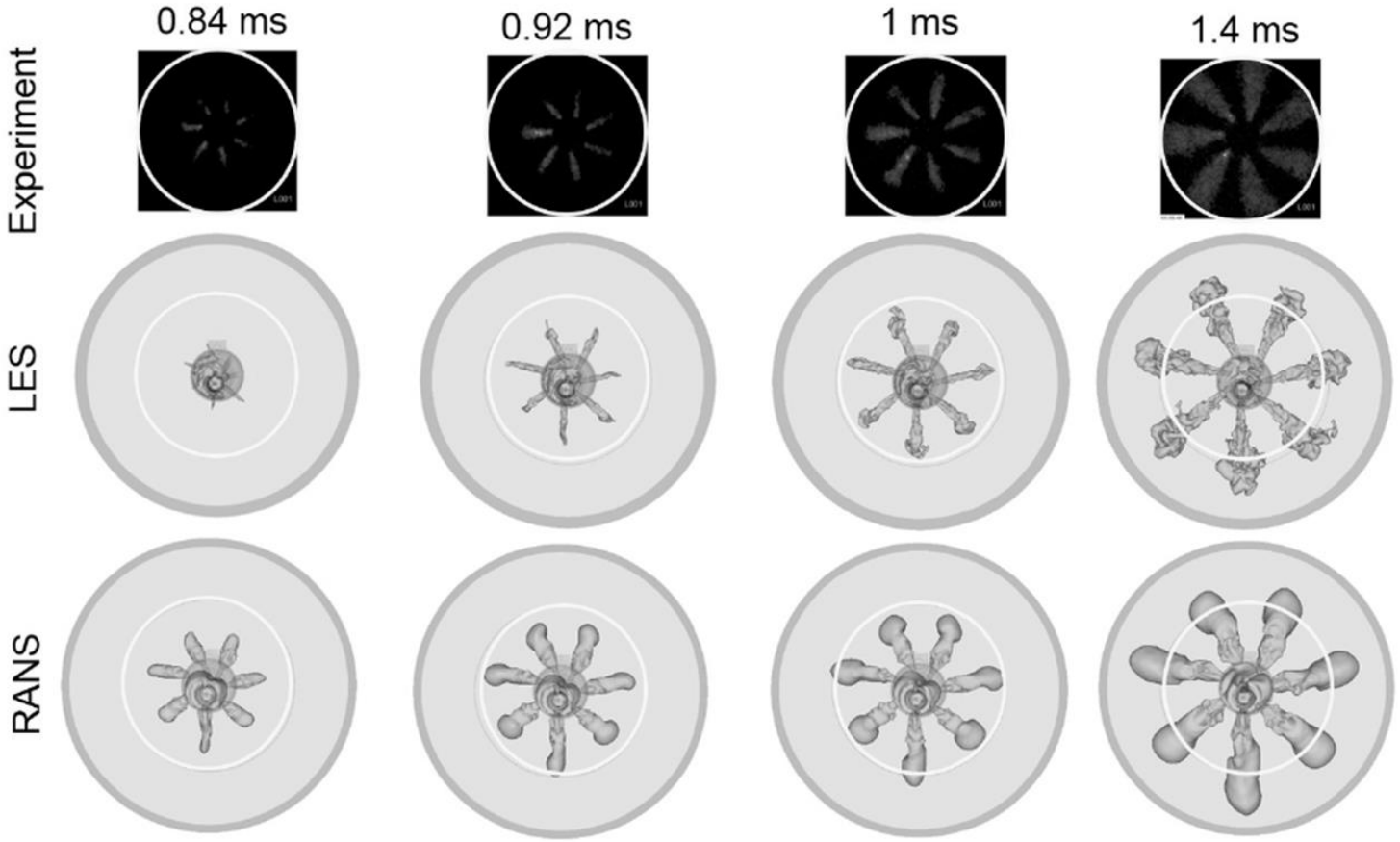


Shapiro, E., Tiney, N., Kyrtatos, P., Kotzagianni, M. et al., "Experimental and Numerical Analysis of Pre-Chamber Combustion Systems for Lean Burn Gas Engines," SAE Technical Paper 2019-01-0260, 2019, doi:10.4271/2019-01-0260.

Case study: CNG PCI Development

- ✓ LES data – OpenFOAM v4.x, 20 realisations, 0.125mm in pre-chamber
- ✓ RANS – VECTIS, k-e TSB, mesh 0.18mm in pre-chamber
- ✓ Calibrated RANS combustion produces comparable results in flame jet propagation and timing

PC-A

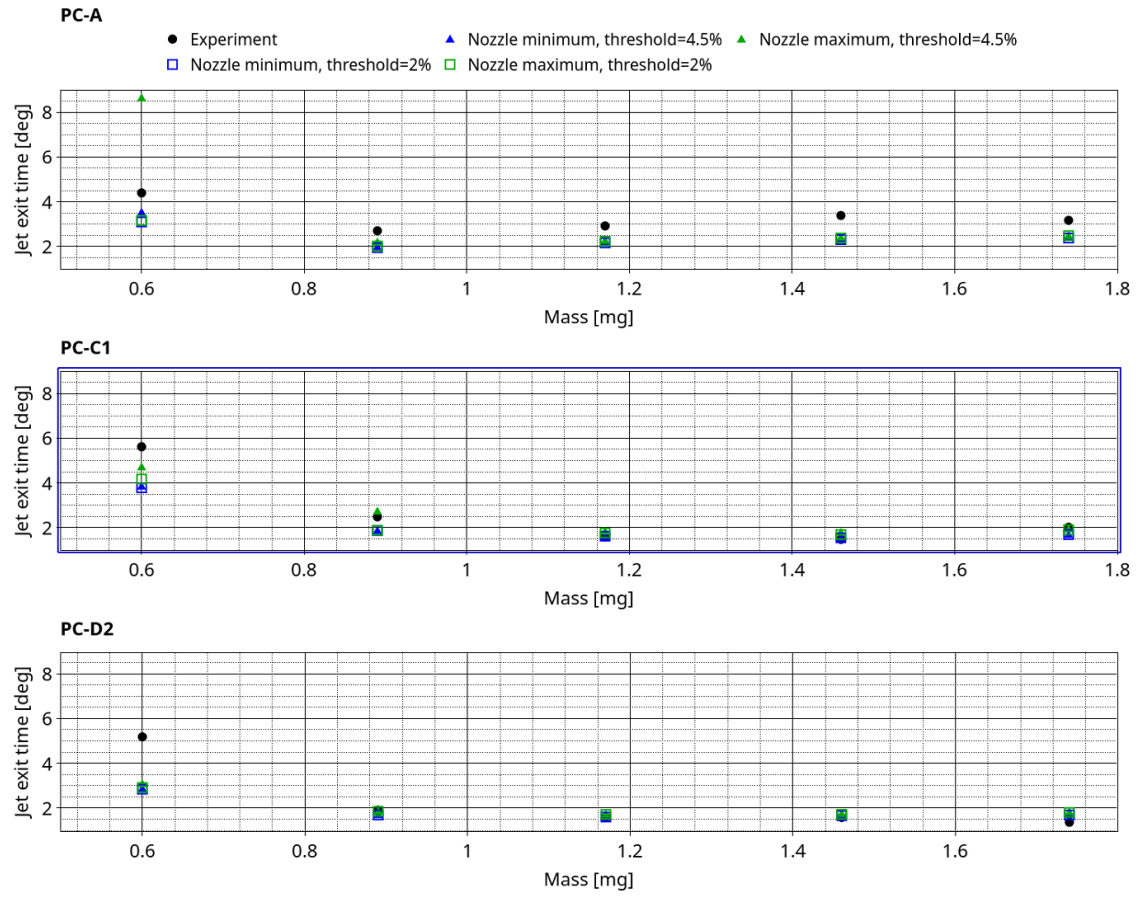


Bolla, M., Shapiro, E., Tiney, N., Kyrtatos, P. et al., "Numerical Simulations of Pre-Chamber Combustion in an Optically Accessible RCEM," SAE Technical Paper 2019-01-0224, 2019, doi:10.4271/2019-01-0224.

http://gason.eu/

Case study: CNG PCI Development

- ✓ The jet exit times are predicted well, with little sensitivity to the threshold value.
- ✓ The overall tendency in the simulation is to result in faster jet exit times than in the experiment.
- ✓ Pre-chamber PC-D2 shows less sensitivity to threshold (less diffuse flame front) and faster flame propagation.

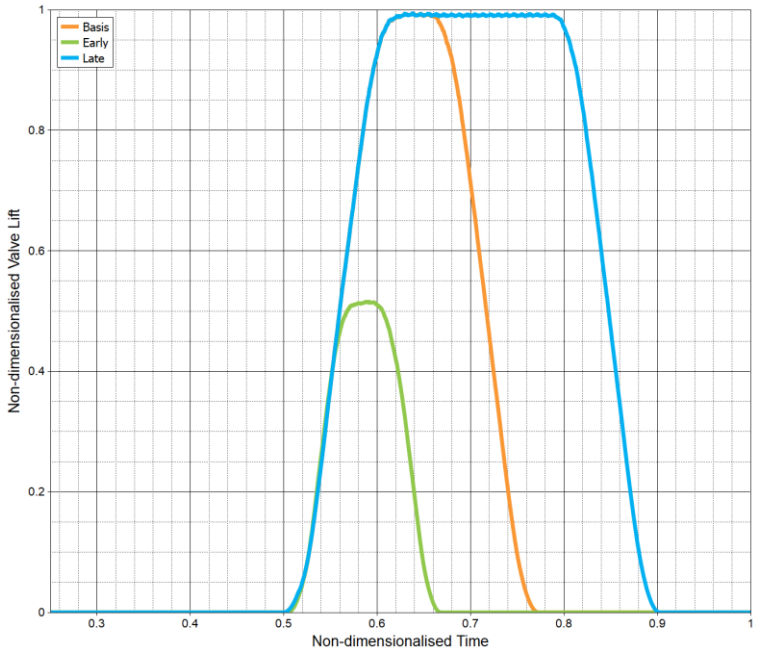


Calibrate once for a baseline, apply for all parametric variations

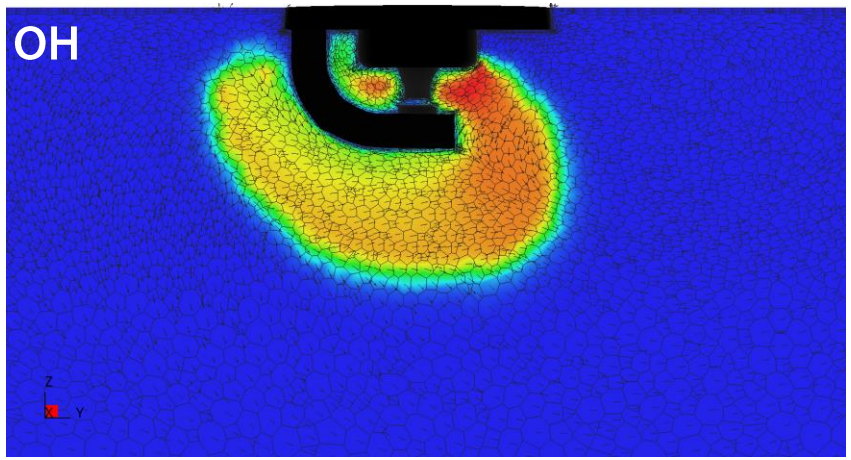
- ✓ Run-times constraints met < 6k core-hours

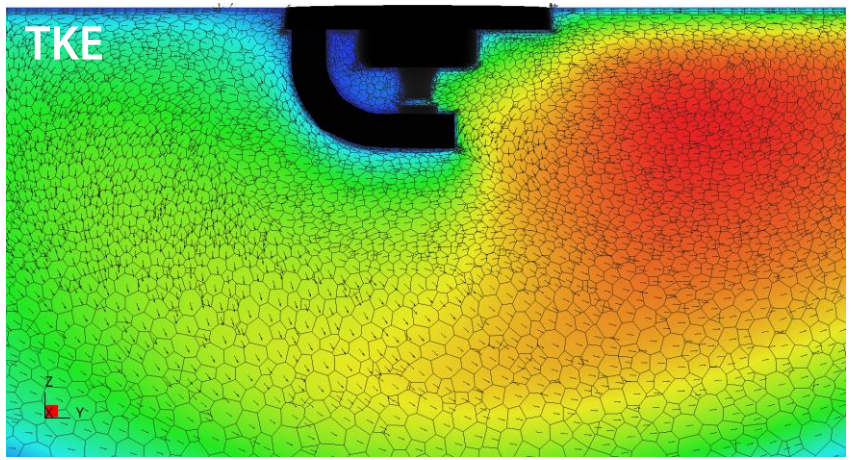
Shapiro, E., Tiney, N., Kyrtatos, P., Kotzagianni, M. et al., "Experimental and Numerical Analysis of Pre-Chamber Combustion Systems for Lean Burn Gas Engines," SAE Technical Paper 2019-01-0260, 2019, doi:10.4271/2019-01-0260.

Case study: Representative Heavy-Duty Engine

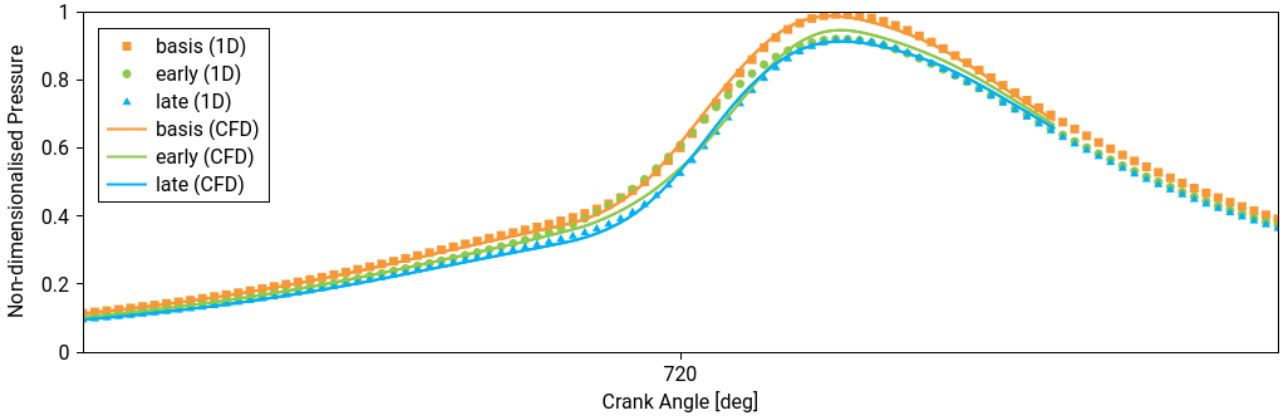


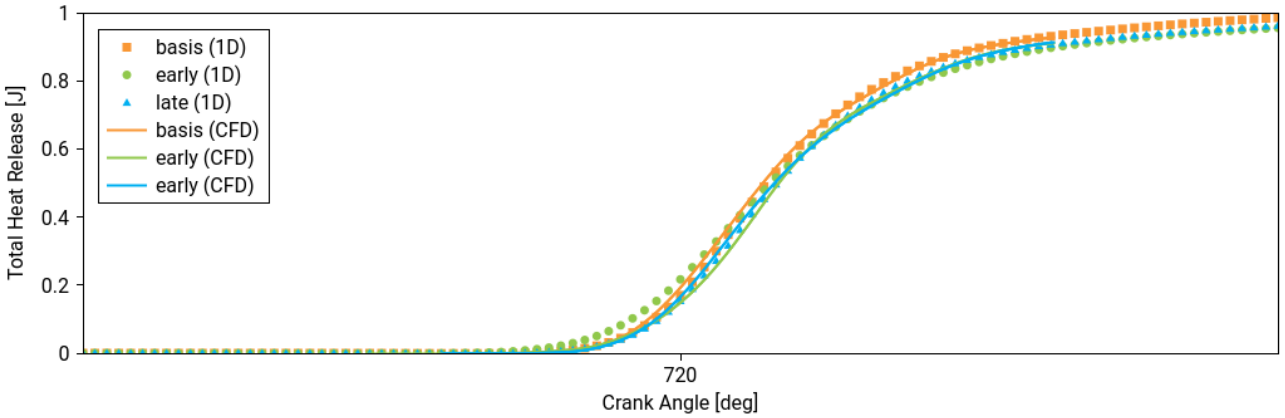
- ✓ Representative Heavy-Duty Natural Gas engine from a major OEM
- ✓ Valve opening timings are a typical parameter varied in the calibration process
- ✓ Valve opening timings **substantially** affect in-cylinder turbulence and, as a result – combustion process.
- ✓ 2 engine configurations with 3 different intake valve timings
- ✓ Polyhedral mesh with boundary layer resolution
- ✓ **Objective:** Demonstration of the approach - model calibration on the basis case yields calibrated combustion model which produces correct design decisions for all three cases





Heavy-Duty Engine: Tabulated Kinetics (CPV)





6-8k core-hours/cycle

- ✓ **Combustion Model:** Combustion Progress Variable (CPV) – Tabulated 0-D reactors with detailed chemistry. G-equation/G variance model used for flame front tracking
- ✓ **Chemical mechanism:** GRI-Mech 3.0 used for CPV and laminar flame speed tables
- ✓ **Spark-ignition model:** Isothermal Discrete Particle Ignition Kernel (DPIK)
- ✓ **Laminar flame speed:** Tabulated using computations of freely propagating laminar flames
- ✓ **Turbulent flame speed model:** Peters' (b1=2, **cm2=1**)
- ✓ **Turbulence model:** k-e Turbulence Scale Adapted
- ✓ **Computational Mesh:** Polyhedral grid with boundary layer
- ✓ **Correct judgement:** centre of combustion and peak pressure

Case/Parameter	Baseline	Early	Late
Peak Pressure Value (Mpa vs Test)	-0.5%	-2.8%	0.7%
Peak Pressure Location (deg vs Test)	-0.8	0	-0.3

Case study: R2DK Development

- The Favre-averaged Navier-Stokes, energy, mass and species fractions are solved,

$$\frac{\partial \bar{\rho}\tilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_j}\left[\bar{\rho}\tilde{Y}_k\tilde{U}_j\right] = \overline{\dot{\omega}_k} + \frac{\partial}{\partial x_j}\left[\bar{J}_{k,j} + J^t_{k,j}\right]$$

- The turbulent quantities are computed using RANS turbulent models (in VECTIS $k{-}\varepsilon$ family is preferred)
- The species production rates and the heat release are computed directly by the LOGEsoft external chemical solver from the mean quantities using any detailed chemical mechanism,

$$\overline{\dot{\omega}_k} = \dot{\omega}_k\left(\bar{T}, \tilde{Y}_k\right)$$

  - Internal sub-stepping is used to march the solution in time and avoid under/over-shoots of the species mass fractions
  - ODE solver with Backward Differentiations Formulas (BDF) predictor-corrector
  - 0D constant pressure reactor assumption
  - The species production/destruction rates used by VSOLVE are estimated by the simple rate expression :

$$\overline{\dot{\omega}_k} = \frac{Y_k^{n+1} - Y_k^n}{\Delta t}$$

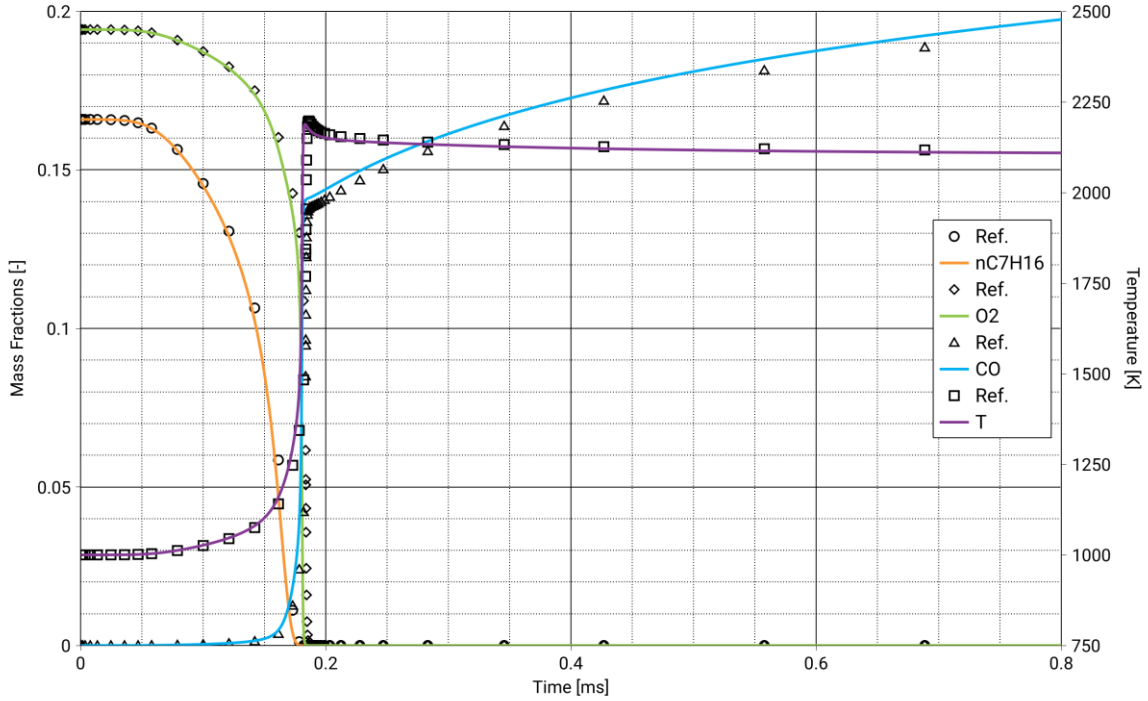
- Main calibration parameter :
  - Arrhenius pre-multiplier for all reactions (C_{user}, with default value 1.0)

$$K_j = C_{user} A_j T^{\beta_j} exp\left(-\frac{E_j}{RT}\right)$$

Case study: R2DK Development

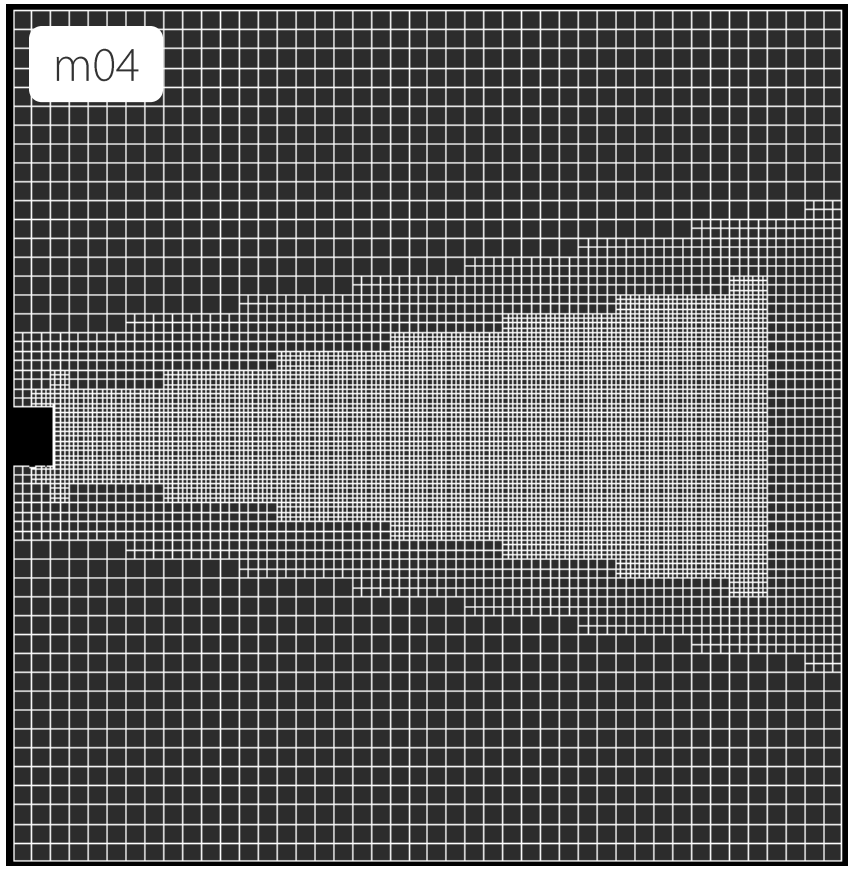
- **Validation** against online chemistry solution (Cantera)
  - 0D constant volume reactors comparison
    - nC_7H_{16} computed with Zeuch mechanism (121 species including PAH, 967 reactions), 60 atm, 1000K and eqr = 3
  - 1D laminar flame speed propagation measurements at STP conditions
    - CH_4 flame computed with the 2sCM2 global mechanism (6 species, 2 reactions)
    - iC_8H_{18} flame computed with the SIP 2.0 mechanism (86 species, 463 reactions)

Cell size [mm]	s_l^0 (CH_4) [m/s] *Ref = 0.384*	s_l^0 (iC_8H_{18}) [m/s] *Ref = 0.30*
0.04	0.360	0.276
0.08	0.378	-
0.16	0.392	-
0.32	0.463	-
0.64	0.501	-



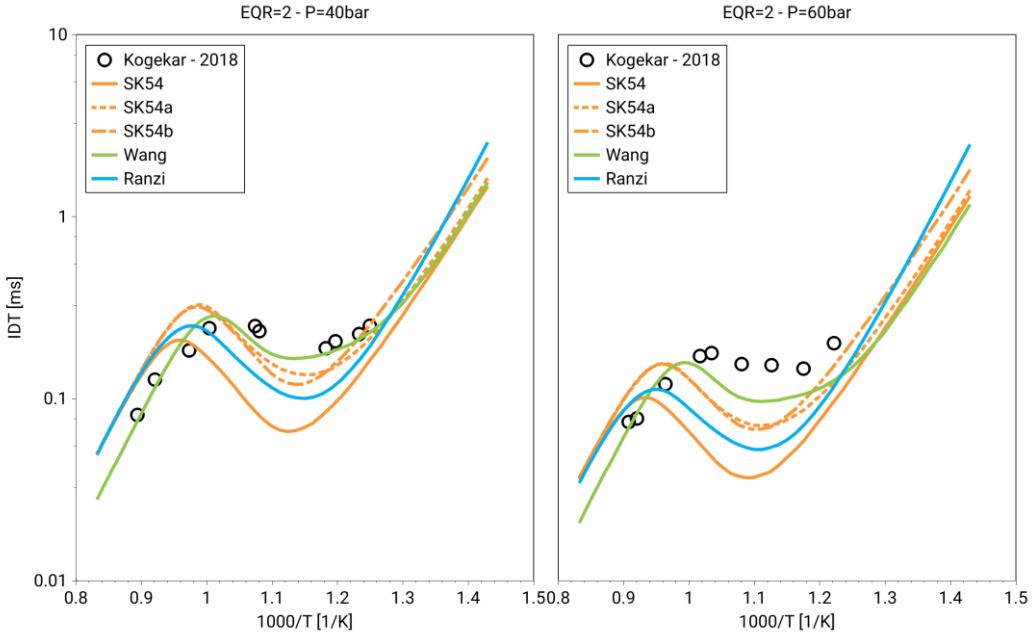
Case study: R2DK Development

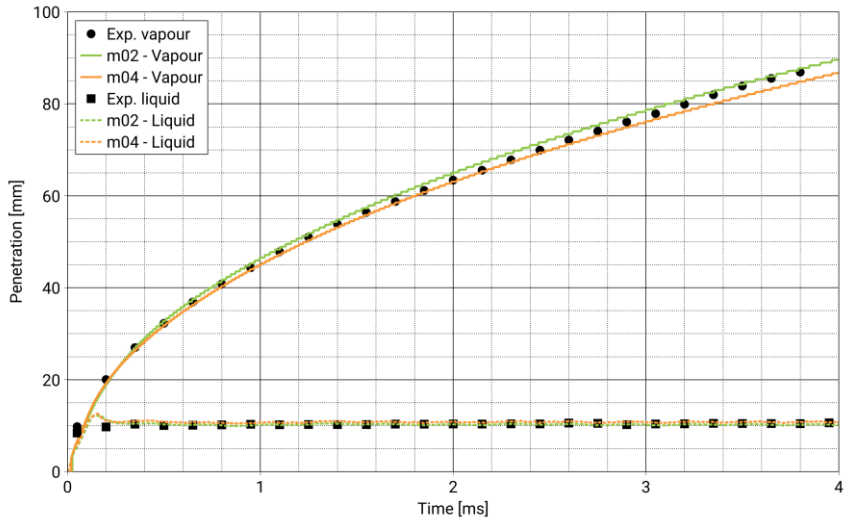
- **Validation** on academic test cases - ECN Spray A n-dodecane flame with ambient temperature sweep
- Measurements available at inert and reacting conditions for validation of spray and combustion
- Sweeps at different conditions simulated using a single calibration
  - $P_{inj} = 150\ MPa$
  - $T = 800, \mathbf{900}, 1000, 1100, 1200\ K$
  - $X_{O_2} = 0.15$
  - $\rho = 22.8\ kg/m^3$
- Computational domain
  - m02 : 2.4mm base grid with 2 levels of refinement (1M cells)
  - m04 : 1.8mm base grid with 2 levels of refinement (500k cells)
- Process of analysis
  - The case is set-up and for the 900K condition
  - Calibration based on Ignition Delay Time (IDT)



Case study: R2DK Development

- **Calibration** of the spray parameters for matching experimental liquid/gas penetrations
- **Choice** of the chemical mechanism
  - SK54 : Yao[1] (54 species / 269 reactions) (best cost/accuracy compromise)
  - Wang[2] (100 species / 432 reactions)
  - Ranzi[3] (130 species / 2395 reactions)
  - Calculations with **Ricardo R-Flame**



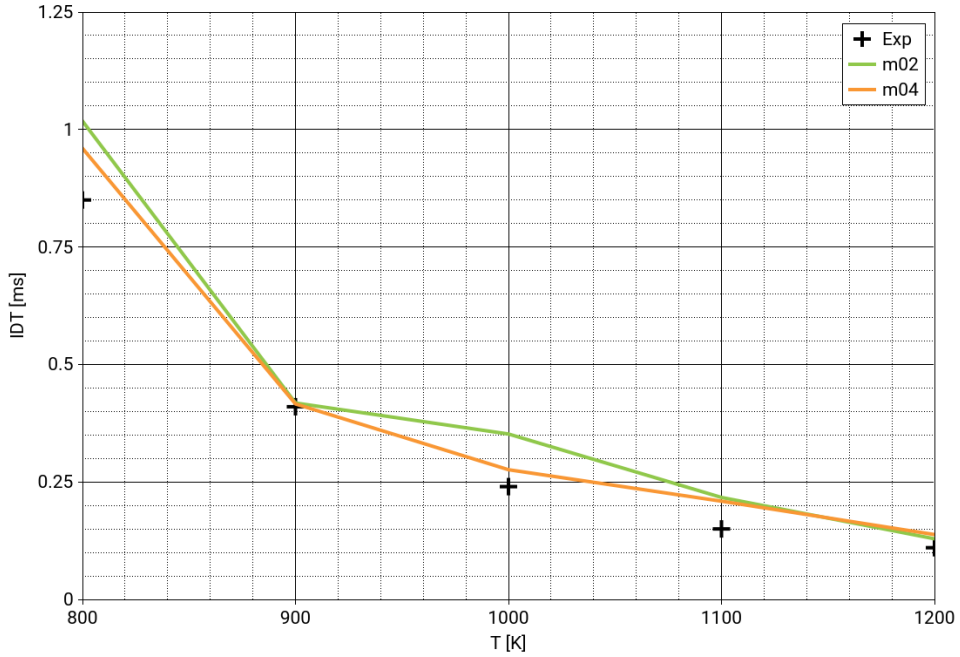


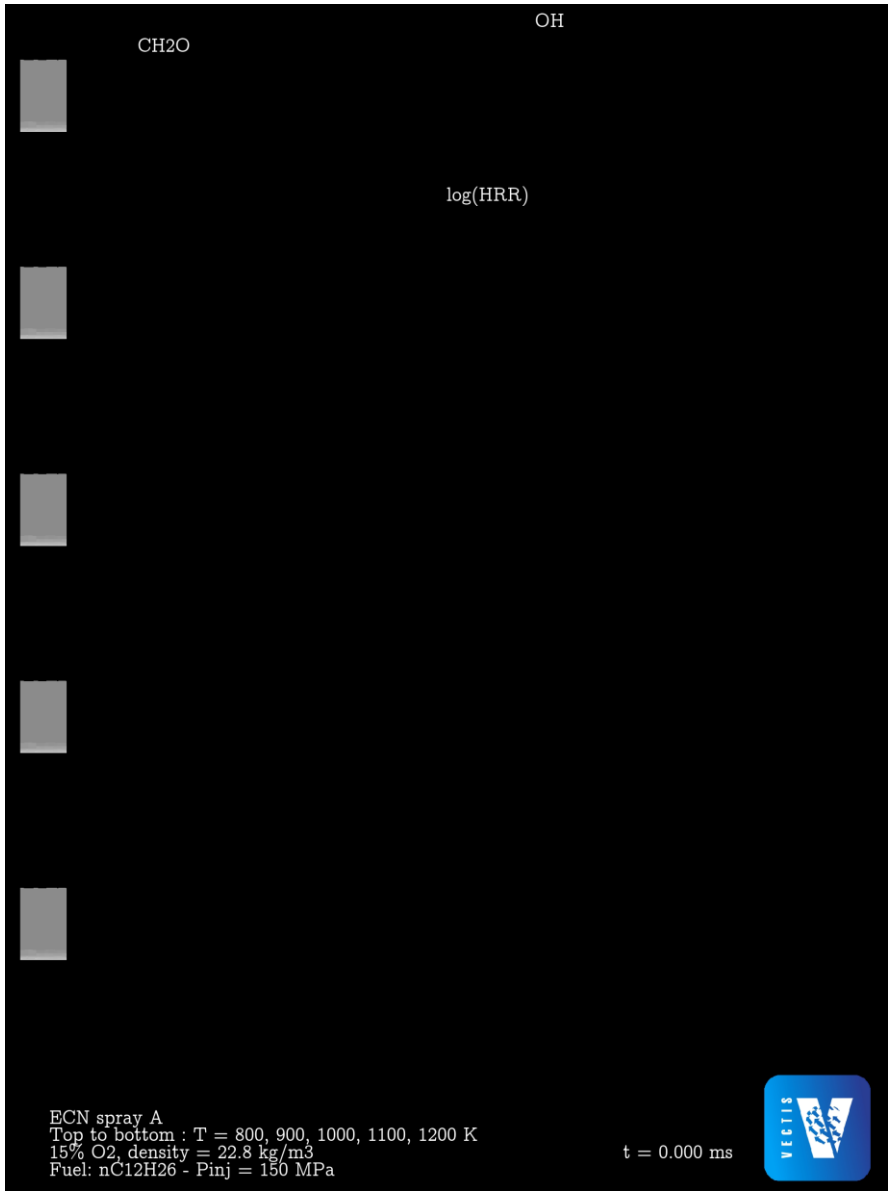
[1] Yao, T. et al. (2017), A compact skeletal mechanism for n-dodecane with optimized semi-global low-temperature chemistry for diesel engine simulations, Fuel 191, pp.339-349
[2] Wang, H. et al. (2014), Development of a reduced n-dodecane-PAH mechanism and its application for n-dodecane soot predictions, Fuel 136, pp.25-36
[3] Ranzi, E. et al. (2014), Reduced Kinetic Schemes of Complex Reaction Systems: Fossil and Biomass-Derived Transportation Fuels, International Journal of Chemical Kinetics 46(9), pp.512-542

Case study: R2DK Development

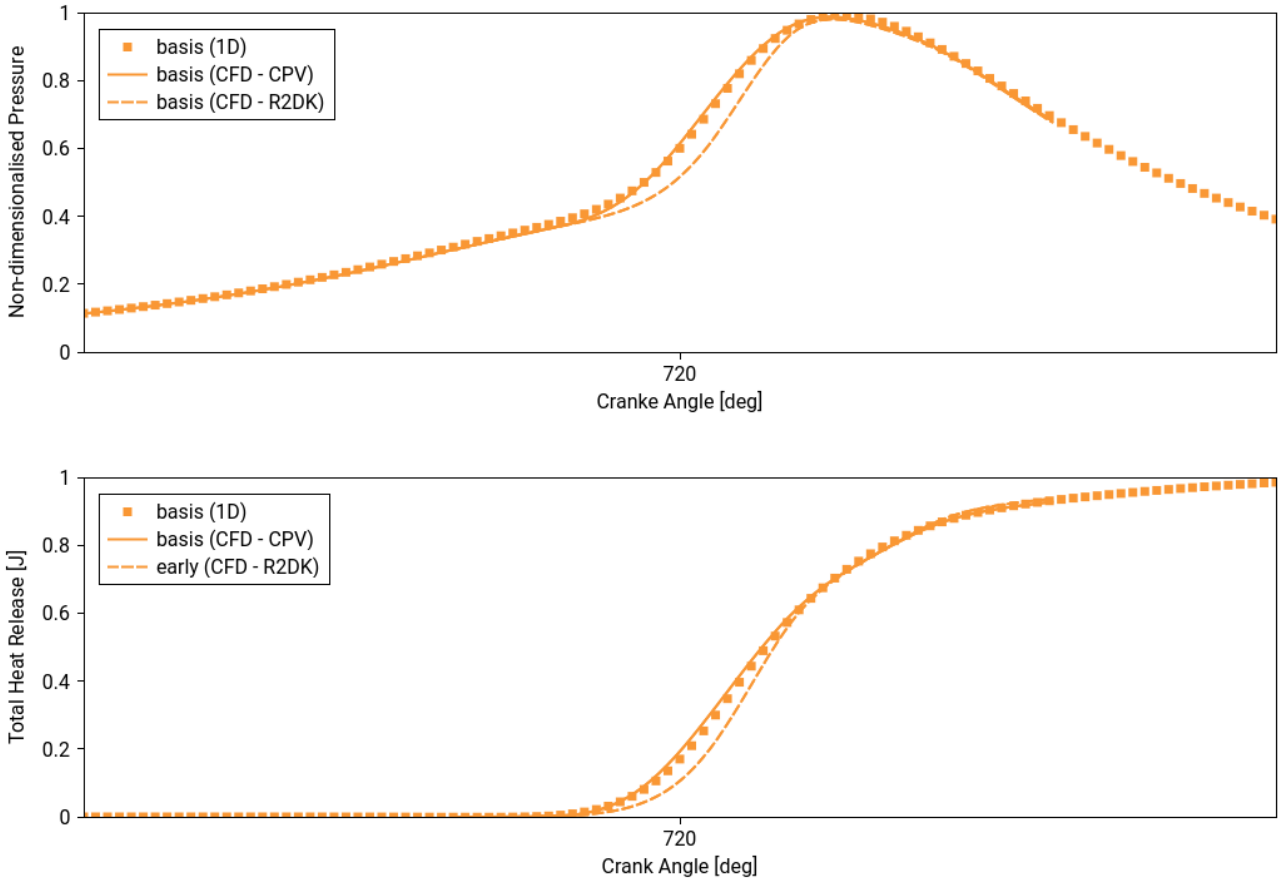
- **Calibration** of the combustion for the case with $T_{ambient}$ = 900 K
  - Change the constant C_{user} to match the exp. IDT value for each grids
  - Exp. IDT : 0.41 ms
  - IDT measured at $\max(dT_{max}/dt)$

- **Computation** of the temperature sweep





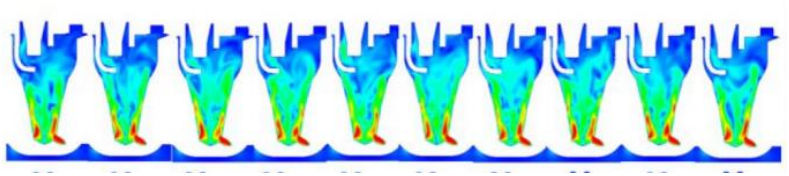
Heavy-Duty Engine: Detailed Kinetics (R2DK)

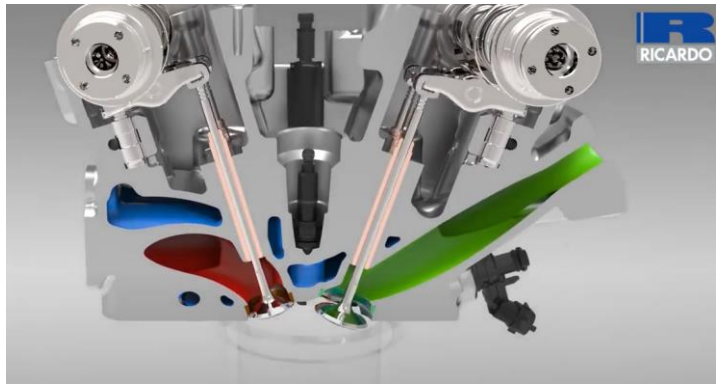


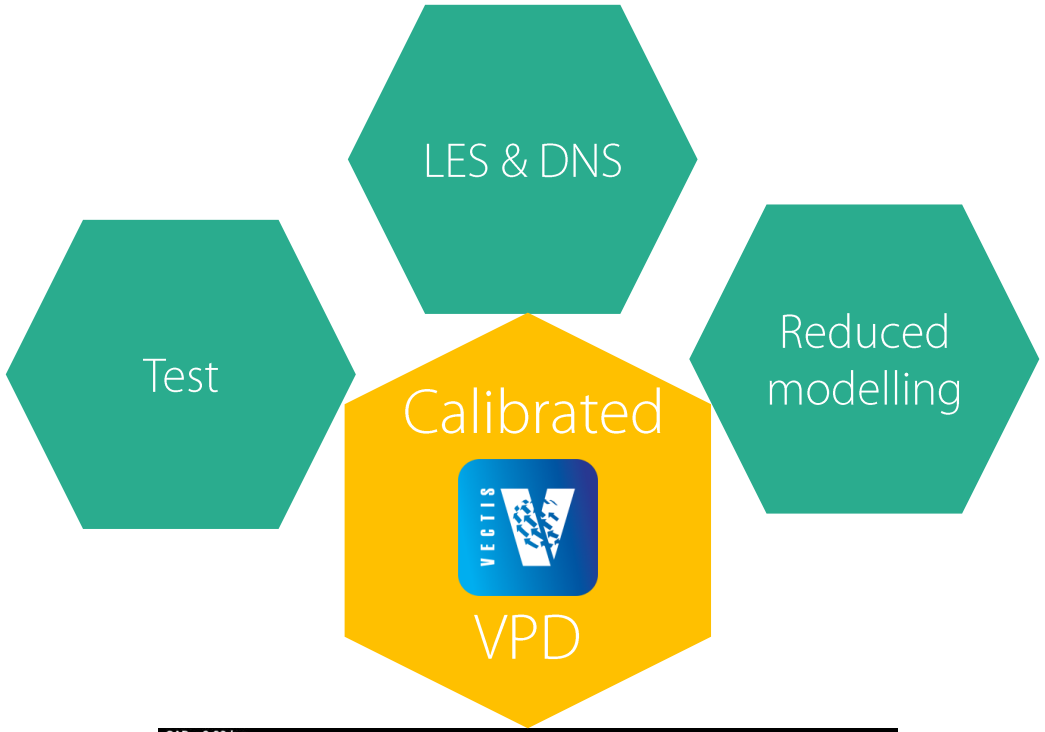
- ✓ **Combustion Model:** Ricardo Detailed Direct Kinetics (R2DK)
- ✓ **Chemical mechanism:** DRM 19 (reduced reaction sets based on GRI-Mech 1.2 with 19 species and 84 reactions)
- ✓ **Spark-ignition model:** Energy deposition
- ✓ **Turbulence model:** k-e Turbulence Scale Adapted
- ✓ **Computational Mesh:** Polyhedral grid with boundary layer
- ✓ **Detailed spark modelling required.**

2k core-hours/combustion event (spark to 25deg), no clustering

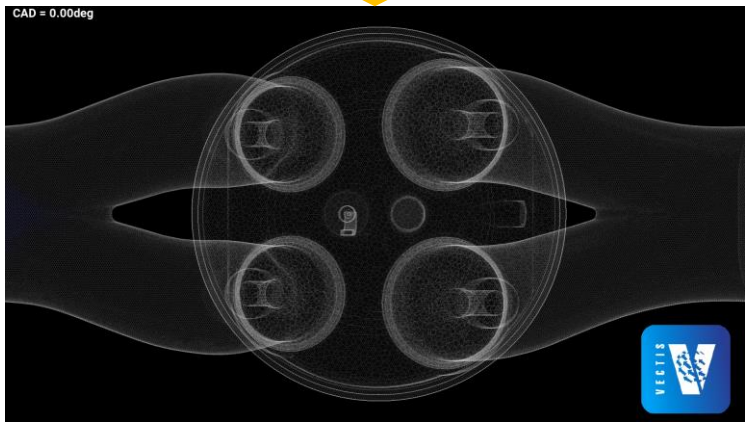
Outlook







$$\begin{cases} \frac{dr_k}{dt} = Q_{r,f} + Q_{r,e} + Q_{r,c} \\ \frac{dT_k}{dt} = Q_{T,W} + S_{T,f} + Q_{T,c} \end{cases}$$



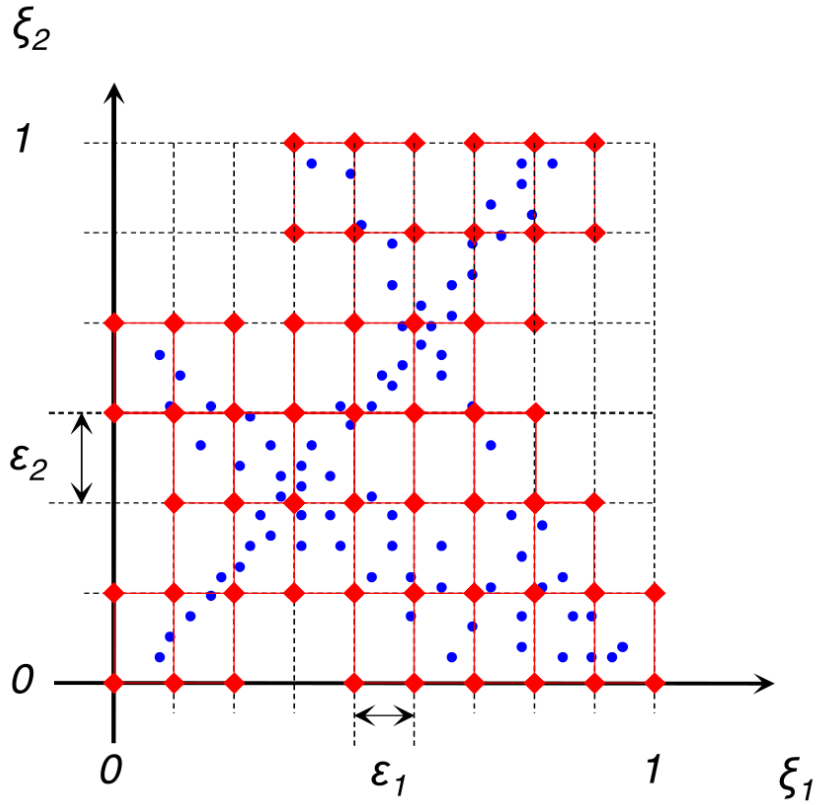
Contact: Evgeniy.Shapiro@ricardo.com

Additional information

Case study: R2DK Development

- **Clustering** method for chemistry computation acceleration[1-3] :
  - Avoid calculating kinetics in cells that have common properties multiple times
  - Cells are grouped in clusters sharing near-identical parameters (mapping step)
  - Kinetics are advanced in each clusters using the mean thermochemical properties
  - The reaction rates are then re-mapped to each cell to account for the difference between the cell and cluster thermochemical state (re-mapping step)
  - Different algorithms available for the mapping/re-mapping steps

- Computation time for a diesel bowl geometry
  - ~185k cells on 24 cores
  - n-heptane mechanism with 121 species and 967 reactions with PAH chemistry
  - Without clustering : ~ 15h
  - With clustering : ~ 9h



[1] Perlman et al. (2012), A Fast Tool for Predictive IC Engine In-Cylinder Modelling with Detailed Chemistry, SAE
[2] Perini (2013), High-dimensional, unsupervised cell clustering for computationally efficient engine simulations with detailed combustion chemistry, Fuel 106, pp.344-356
[3] Babajimopoulos et al. (2005), A fully coupled computational fluid dynamics and multi-zone model with detailed chemical kinetics for the simulation of premixed charge compression ignition engines, Int. J. Engine Res. 6, pp. 497-512