Virtual Engine Test Bench Digital Twin — Proof of Concept Summary

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Three proof-of-concept studies were developed to demonstrate an integrated multi-fuel digital-twin framework that combines physics-based combustion modelling with machine-learning-driven correction, in alignment with the DT-HATS DC14 objectives. All simulations (excluding the OpenFOAM-based CFD analysis) were conducted using the author's existing Virtual Engine Test Bench model, which has been further extended and refined specifically for this application.

1) Multi-Fuel Combustion Behaviour

Objective: Evaluate the combustion characteristics of gasoline, hydrogen, ammonia, and a hydrogen–ammonia blend (10 % H_2 by mass) at 3000 rpm under wide-open-throttle (WOT) conditions to assess lean-limit performance and fuel-specific IMEP behaviour.

Methodology:

- Single-zone Wiebe-function combustion model.
- Rich to lean operation ($\lambda = 0.8 – 1.5$).
- Beyond $\lambda \geq 1.3$, combustion duration fixed to maintain numerical stability.
- Fuel thermochemical properties and laminar flame-speed correlations defined individually for each fuel.

Results Summary:

- Hydrogen delivered the highest IMEP (15.6 bar at $\lambda = 0.8$) and retained stable operation up to $\lambda = 1.5$, supported by its high laminar flame speed (≈ 1.2–1.5 m/s) and strong turbulence interaction.
- Gasoline produced intermediate IMEP (13.4 bar at $\lambda = 0.8$) with a near-linear decline toward lean conditions, consistent with its moderate flame speed (~0.2 m/s).
- Ammonia showed the lowest IMEP (13.2 bar at $\lambda = 0.8$) due to inherently slow chemical kinetics (laminar flame speed < 0.05 m/s).
- 10 % H_2–NH_3 blend demonstrated a marked "stabilised-ammonia" effect, increasing IMEP by ~30 % relative to pure ammonia and extending stable combustion to leaner mixtures.
- The correlation between flame-speed hierarchy (H_2 > H_2–NH_3 > Gasoline > NH_3) and IMEP confirms the kinetic-limited nature of ammonia combustion and highlights the potential of hydrogen enrichment to mitigate slow-flame propagation and expand the lean-limit envelope.

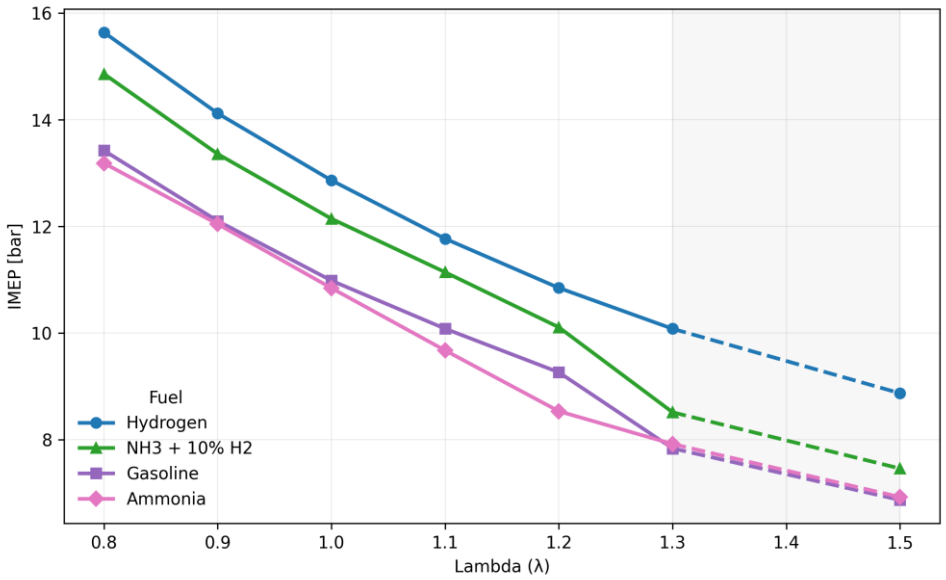

Figure 1: IMEP vs Lambda for Gasoline, Hydrogen, Ammonia, and 10 % H_2–NH_3 blend at 3000 rpm / WOT (dashed region denotes fixed burn duration beyond $\lambda \geq 1.3$)

2) Machine-Learning Correction

Objective: Reduce model–dyno torque error by learning small, physically-constrained residual corrections to mixture, friction and phasing.

Methodology:

- Inputs: Engine speed and a VVL/VVT flag.
- Outputs (learned residuals):
  - Δλ (small lambda bias applied to fuelling to match observed load at WOT),
  - ΔFMEP (friction offset),
  - ΔSOC (spark/combustion start correction).
- Training: SPSA optimiser on steady WOT sweep (1000–7000 rpm)
  - loss = torque error + smoothness + monotonicity penalties (ΔFMEP increases with rpm; bounded Δλ, ΔSOC).
- Deployment: Residuals added on top of the physics model (grey box).

Results Summary:

- Torque accuracy: The ML-corrected model reproduces dyno torque within ±2 % across most of the operating range (1000–6200 rpm), compared to 3–7 % baseline error.
- ΔSOC: ~+1 CA° advance around the VVL/VVT transition, improving high-rpm torque retention.
- ΔFMEP: Monotonic increase with rpm, consistent with mechanical losses; this absorbs unmodelled friction trends.
- Δλ: Small, smooth bias that refines load in the upper range while respecting knock and stability limits.
- Corrections are smooth and physically plausible; the underlying physics model remains interpretable.

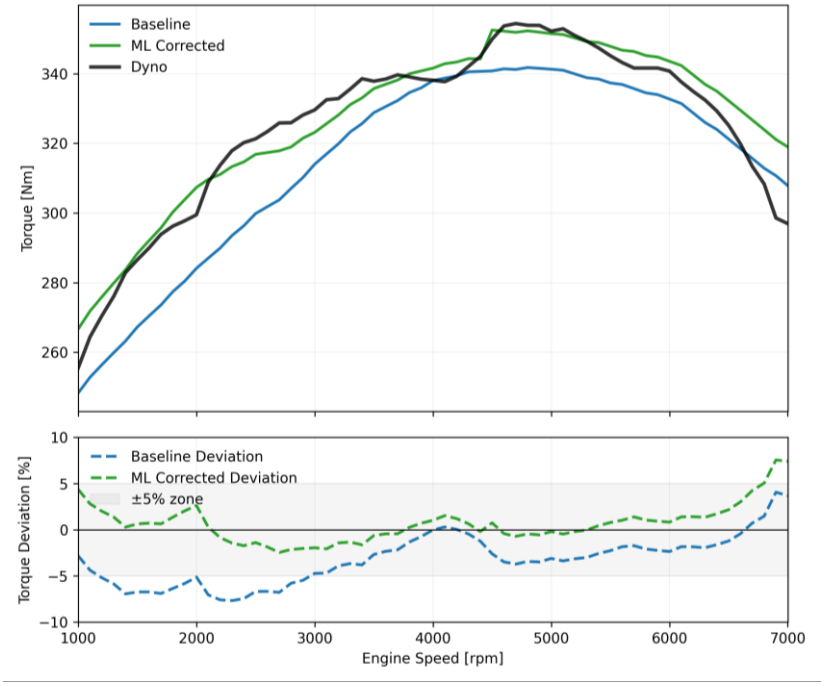

Figure 2: (Top) Torque vs RPM for Baseline, ML-corrected , Dyno. (Bottom) Torque deviation vs RPM: Baseline and ML-Corrected vs Dyno (axis zoomed to highlight ±5 % band)

3) CFD-Informed Combustion Update

Objective: Demonstrate how coupling CFD-derived mean unburned-gas temperature and turbulence kinetic energy fields into the combustion model influences flame-speed and phasing behaviour within the Virtual Engine Test Bench.

Methodology:

- Hydrogen compression within the combustion chamber was simulated in OpenFOAM, and volume-averaged unburned-gas temperature and turbulent kinetic energy were extracted from the flow field.
- These values were stored as a function of engine speed (1000–7000 rpm) and imported into VTEB via a CFD adapter module.
- The combustion_Wiebe() function was extended to accept $\bar{T}_{(u)}$ and $\bar{k}$ as additional inputs, allowing dynamic adjustment of laminar and turbulent flame speed.
- The simulation was repeated across the full speed range to quantify changes in torque and turbulent flame speed relative to the baseline.

Results Summary:

- The CFD coupling leads to visibly faster burn rates at mid-range speeds due to elevated turbulence intensity ($\bar{k}$), while retaining smooth behaviour near the clipping limit (S_T ≈ 60 m/s).
- This demonstration does not represent a validated study; the objective is to illustrate the functional coupling of low and high-fidelity domains and how CFD-derived parameters can enrich the combustion modelling workflow.

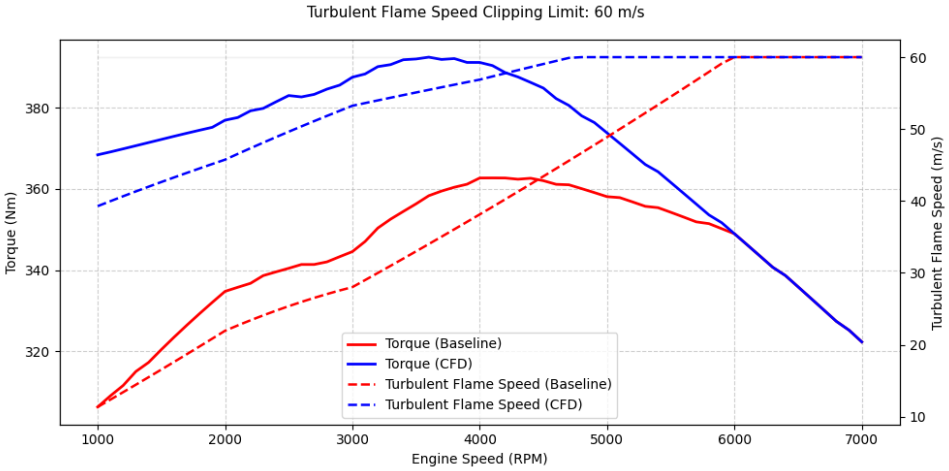

Figure 3: Torque and turbulent-flame-speed comparison between baseline and CFD-coupled models

4) **Conclusion**

This proof-of-concept demonstrates a multi-fidelity digital-twin framework that integrates:

- Physics-based modelling: combustion thermochemistry and system-level performance prediction.
- Data-driven correction: machine-learning residuals to capture unmodelled effects.
- CFD coupling: turbulence and thermal inputs for high-fidelity calibration and model enrichment.

Together, these three demonstrations form a grey-box digital-twin prototype that merges physical combustion modelling, data-driven adaptation and CFD-derived corrections. The approach establishes a scalable workflow for developing interpretable, data-efficient digital twins for sustainable-fuel engine systems.