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# Evaluating the transient performance of a direct injection of a natural gas engine using a phenomenological combustion model

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**Abstract**

Significant near-term reductions in greenhouse gas emissions from commercial vehicles can be achieved by combining technology advances, including powertrain hybridization and engine efficiency improvements with low-carbon fuels such as natural gas (NG). NG can reduce greenhouse gas (GHG) emissions by 15%-20% compared to diesel when burned in a diesel-like pilot-ignited, direct injection of NG process. Combining advanced NG engines with vehicle hybridization offers substantial GHG reduction potential but needs to be evaluated over real-world driving conditions. Developing an optimized hybrid system requires simulating engine and vehicle on various real-world duty cycles. This paper presents a development of a 1-D model which adapts GT-SUITE's phenomenological DI-Pulse predictive model to simulate a 6-cylinder pilot-ignition, direct injection of NG engine. A single set of parameters were obtained for the combustion calibration. The model is then used to assess performance over a transient drive cycle to provide a qualitative assessment of the emissions penalties of transient operation. The model showed an average error of less than 5% in the steady operation. Cumulative errors of fuel consumption and nitrogen oxide (NOx) emissions in transient cycles were less than 2% and 10%, respectively. The proposed NOx transient penalty estimation method showed that the NOx penalty share was 11% of the total NOx emissions emitted in the WHTC cycle. These results suggest that the developed model provides an acceptable accuracy in its predictions and can be used in engine evaluation studies, especially when combined with new technologies like hybrid powertrains across different operating conditions and duty cycles.

## 1. Introduction

Long-haul goods transportation poses a substantial challenge to the decarbonization of transportation. In Canada, greenhouse gas (GHG) emissions from heavy-duty vehicles (HDVs) have tripled since the mid-1990's [1]. Amongst HDVs, tractor-trailers (class 8 commercial trucks) emit a significant part of greenhouse gases (GHGs) and nitrogen oxides (NOx) emissions. Although class-8 trucks form 9% of the commercial vehicles fleet in the U.S., they emit almost half of the NOx and GHGs [2]. These vehicles must meet stringent NOx and GHG emissions regulations. In Europe, HDV $CO_2$ reductions are to be 45% in 2030, 65% in 2035, and 90% in 2040 compared to 2019 levels [3], [4]. In North America, new legislation is expected to drive further reductions in NOx emissions [5]. These regulatory challenges and the urgent need to achieve substantial reductions in GHG emissions have driven investigations into engine, vehicle, and fuel technologies. Combining high-efficiency engines with low-carbon fuels and a hybrid-electric powertrain has the potential to reduce emissions. Assessing the potential benefits of this approach at an early stage of development depends on predictive models of engine performance using low-carbon fuels when run over engine duty cycles defined based on a hybrid powertrain in a real-world driving environment.

Various technological approaches are being developed to reduce the environmental impact of HDVs and to meet these regulatory requirements. For example, in the US Department of Energy's SuperTruck II program, original equipment manufacturers have demonstrated 100% improvement in vehicle freight efficiency (on a ton-mile-per-gallon basis) relative to a 2009 baseline and peak brake thermal efficiencies (BTEs) approaching 55% at 65 mph (104 km/h) on a dynamometer [6], [7]. SuperTruck II program and similar studies have shown that hybridized powertrain is an

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important contributor to the further reduction of $CO_2$ in commercial vehicles [6],[7]. Combining engine and vehicle technologies with the hybrid powertrain further improves fuel economy and is essential in complying with emission regulations [8]. Also, hybrid powertrains with the electric motor's assistance can reduce the engine's dynamic response in transient operation, which has been shown to decrease NOx emissions at the cost of added small fuel penalty [9]. Since the map-based engine data misses the transient effect [10], it is advantageous to quantify the transient operation impact on emissions in different hybrid powertrain configurations. However, little work has been done to study the transient dynamics of the engine and associated emissions when simulating the behaviour of a hybrid vehicle, and none has proposed a general methodology to consider the penalty factors. The previous studies for penalty factor development required several experimental tests involving costly facilities, such as dynamometers and fast-response exhaust gas measurement devices.

Combining these high-efficiency engine and vehicle technologies with a low-carbon fuel such as natural gas offers a pathway to even greater GHG reductions. Directly injected natural gas, injected when the piston is near top-dead-centre and ignited by a diesel pilot that was injected prior to the natural gas, can retain diesel-like efficiency. Through the use of a dual concentric needle injector, the pilot and main gas injections can be controlled independently. Using this approach, many of the advances in diesel engine technology can be carried over to a low-carbon gaseous fuelled engine [11].

The best approach to combining a high-efficiency NG engine with a hybrid powertrain must be evaluated. Appropriate sizing of the powertrain components and prediction of the net GHG benefits depends on an accurate predictive model for an NG-DI engine applicable to different real-world driving cycles. A 1-D simulation allows us to evaluate various combustion strategies and investigate engine and powertrain system sizes over steady-state and transient conditions. This paper presents a 1-D predictive model that adapts GT-Suite's phenomenological DI-Pulse model to simulate the NG-DI combustion and emission in both steady-state and transient operation. Finally, the verified 1-D transient model is shown to be used to evaluate the transient operation and quantify the transient penalties.

## 2. Methodology

The engine that the model in this work is based on is a heavy duty late-cycle direct-injection natural gas engine with pilot ignition. The engine is equipped with a fuel system based on Westport's high pressure direct injection (HPDI) dual concentric needle injectors. Specifications of the engine are provided in Table 1. The engine model is developed in GT-SUITE™ v. 2021. The engine model development included a predictive phenomenological combustion model calibrated for the power cylinder, followed by the development of a multi-cylinder engine that was validated under both steady-state and transient operating modes. Validation was conducted over a range of steady-state and transient points provided by the industrial partner.

### *2.1 Combustion Model Validation (Single Cylinder)*

This study applies GT-Suite's phenomenological DI-Pulse model to simulate pilot diesel and main NG fuel combustion. DI-Pulse can predict the combustion rate and the associated emissions in the engine by discretizing the engine into three zones, including the main unburned zone, spray unburned zone, i.e., fuel and entrained gas, and burned zone, which contains combustion products. The DI-Pulse model has four main sub-models, each containing the related calibration parameter. The sub-models include entrainment, ignition, and premixed and non-premixed combustion.

The model was adapted to allow two distinct fuels to be injected as part of the phenomenological DI-pulse model. The combustion model was calibration at the six modes shown in Fig. 1 using heat-release-based calibration. A Genetic Algorithm (GA) approach was used to optimize the six parameters of the phenomenological combustion model in a single-cylinder model of the multi-cylinder engine. A single set of calibration parameters were obtained, as shown in Table 1, that can be used for all areas of the engine map. Maintaining the constant parameters makes the model predictive and reliable to be expanded to the engine areas outside the calibration zone.

Table 1. DI-Pulse model parameters

| Parameter | Entrainment rate | Ignition delay | Premixed combustion rate | Diffusion combustion rate |
|---|---|---|---|---|
| Value | 0.67 | 1.68 | 0.07 | 0.36 |

### 2.2 *Steady-state Model Development (Six-cylinder Engine)*

After verifying the in-cylinder combustion and heat release model, the developed power cylinder was incorporated into a full six-cylinder engine model. The full engine model includes the six cylinders, intake system, exhaust system, and turbocharger models. Moreover, the extended Zeldovich mechanism was used in the six-cylinder engine model to develop a NOx model. The NOx model includes six different parameters which were calibrated using the GA optimization in the full engine model with the exact engine operating points used in the combustion model calibration.

### 2.3 *Transient Model Development*

A simplified control approach was implemented in GT-Power to simulate the engine in transient operation. A PID controller was embedded in the full engine model to get the transient cycle load demand and adjust the NG injection quantity in the injector to trace the requested torque trajectory. Other injection parameters, such as SOI and pulse width for NG and diesel fuels, were defined as a function of engine speed and torque by interpolating or extrapolating from the available steady-state points. In addition, the fuelling controller (PID) tuning parameters were fixed. Also, the previously developed NOx model was used without any changes in the transient model.

### 2.4 *Penalty Factor Development*

Another application of the transient model was to analyze the NOx emissions of transient ramps in the WHSC cycle during different load shifts. The transient NOx emissions in transient ramps were compared with their corresponding steady-state values to identify any probable deviation (penalty mass) from the steady-state response. The torque and speed of each operating point alongside the engine steady-state NOx map were needed to determine the steady-state NOx response during these ramps. The results of the NOx penalty mass are described in the next section.

### 2.5 *Validation Data*

This study used experimental data from an NG-DI heavy-duty engine (see Table 2) to define and validate the engine model.

Table 2 The industrial partner collected the engine data on a multi-cylinder research engine supporting their technology development activities. Eleven steady-state operating points were collected and are shown in Fig. 1. Six representative points that are particularly important for the in-use operation were selected to develop the model. A further five points were selected to establish the model's ability to operate outside of the range of values where it was calibrated. Transient data was collected at a 0.1 s frequency in both WHTC and WHSC cycles and included intake and exhaust pressure, temperature, and intake air flow measurements, along with fuel flow (NG and diesel). Emissions were measured using an AVL emissions bench measuring undiluted engine-out emissions (i.e., before the after-treatment system).

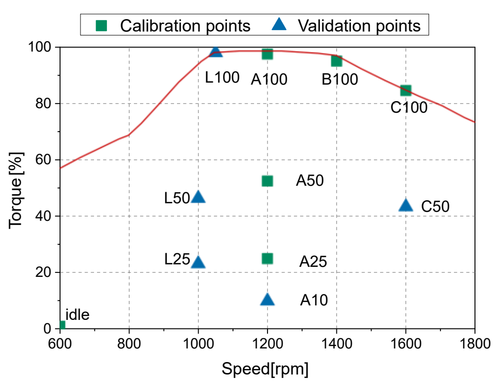



Figure 1. Engine steady-state operating points.

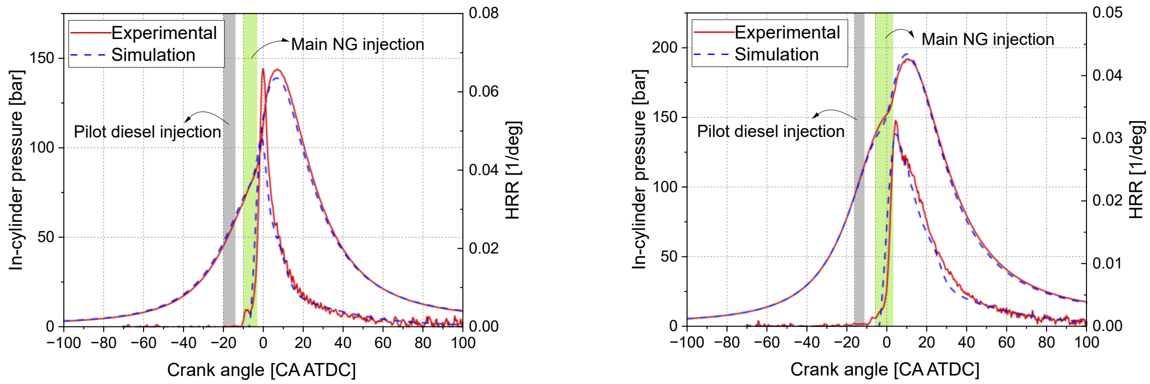
Table 2. Engine specifications

| | |
|---|---|
| Engine configuration | Inline six-cylinder |
| Power per cylinder, HP | 76 |
| Max. BMEP, bar | 23 |
| Fuel system | Direct injection,<br>dual concentric needle HPDI |
| Aspiration | Turbocharged |
| Displacement per cylinder, L | 2.1 |
| Compression ratio | 17:1 |
| Bore × stroke, mm × mm | 131 × 158 |
| After-treatment systems | DOC/ DPF/ SCR/ ASC |

## 3. **Results and Discussion**

### 3.1 *Engine Steady-state Operation*

The power cylinder and engine model provide a good representation of the in-cylinder combustion process. Fig. 3 shows the cylinder pressure and HRR profile for peak power and cruising conditions (A50 and B100 in Fig. 1). The 1-D model shows small errors in both cylinder pressure and HRR that are unlikely to have a relevant impact on the predictions from the combustion model. The model generally performed well at predicting key engine parameters, including fuel consumption, peak cylinder pressure, NOx emissions, flow rates, and exhaust temperature. As would be expected, the calibration points showed higher accuracy than the verification points; but in all cases, errors were small, as shown in Table 3.**Error! Reference source not found.** Predicting BSFC and NOx with good accuracy is essential in hybridization studies to evaluate the hybrid powertrain impact.




(a) (b)

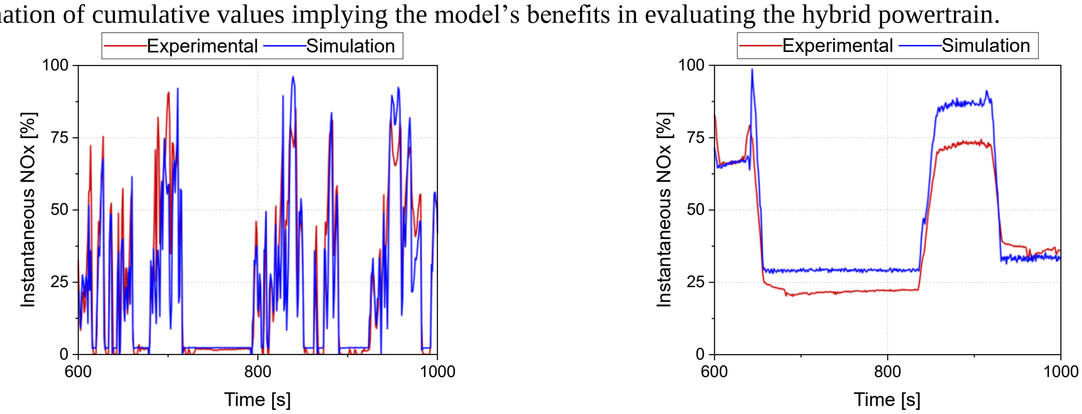
Figure 2. Comparison between experimental and simulation results for in-cylinder pressure and heat release rate in (a) A50 and (b) B100 operating points.

Table 3. The relative error for both calibration and validation steady-state points

| | Average Error (%) | | | | | | |
|---|---|---|---|---|---|---|---|
| Parameter | Torque | BSFC | PCP | NOx | Airflow | Turbine inlet temp. | Turbine outlet temp. |
| Calibration points (n=6) | 2 | 2 | 5.3 | 12 | 2.3 | 2.3 | 2.6 |
| Verification points (n=5) | 4.6 | 4.6 | 3.2 | 14 | 5.7 | 4.4 | 5.2 |

### *3.2 Engine Transient Operation*

The transient model predicted the cumulative fuel consumption with 98% accuracy. Also, the cumulative error for NOx emissions in WHTC and WHSC cycles is 12.9% and 8.5%, respectively. The model followed the NOx responses in both cycles with good accuracy, as it is shown for a segment of cycles in Fig. 4. These results suggest a good estimation of cumulative values implying the model's benefits in evaluating the hybrid powertrain.

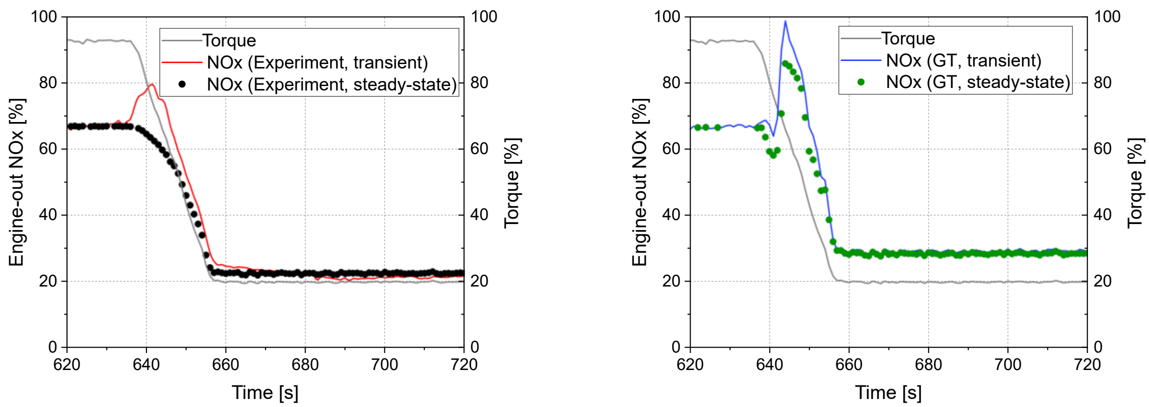



(a) (b)

Figure 3. Comparison between experimental and simulation NOx, (a) for WHTC, and (b) for WHSC

### *3.3 NOx Penalty Factors*

The transient model was used to identify any NOx penalty during transient ramps of the WHSC cycle. Analysis of the transient model over WHSC showed that during tip-out torque profiles, the transient NOx emissions were higher than the associated steady-state response. However, in tip-in profiles, both steady-state and transient responses were coincident. As seen in Fig. 5, both experimental and simulation results showed a transient penalty mass in the same tip-out load change over the WHSC cycle.

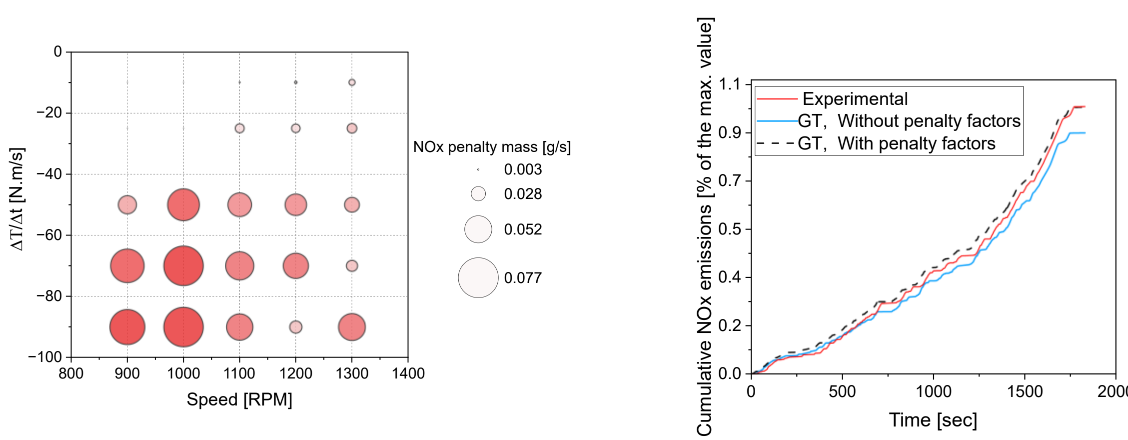



(a) (b)

Figure 4. A segment of the WHSC cycle comparing transient and steady-state responses (a) from experimental test and (b) from simulation.

The model was utilized to define different tip-out torque rates to be simulated at different engine speeds to capture the NOx penalty mass. The torque rates of -10 N.m/s to -90 N.m/s were defined to be examined in the 1-D model to quantify the associated NOx penalty. The main reason for selecting the torque rates in -10 to -90 N.m/s is that the most frequent torque rate changes are in this range in the WHTC cycle. The results of NOx penalty mass are displayed in Fig. 6a where the penalties are higher in sharp tip-out transient while in lower transient rates such as -10 to -20 N.m/s, the penalties are negligible.

The penalty map of Fig.6a is applied to WHTC cycles to quantify and evaluate the penalty share. Also, the penalty mass obtained from the -90 N.m/s torque rate was applied to the higher torque rates. As a result, transient emissions in the WHTC cycle were responsible for 11% of the total NOx, as shown in Fig. 6b.




(a) (b)

Figure 5. (a) NOx penalty factor map obtained from the transient model, and (b) share of the penalty factors in cumulative NOx over the WHTC cycle.

## 4. Conclusions

In this paper, a 1-D model is developed that adapts DI Pulse predictive combustion model to simulate a 6-cylinder NG-DI engine in both steady-state and transient operations. The paper also introduces a simple method for estimating transient emission penalties by using the validated transient model, which is demonstrated on WHTC cycles. The main results of this paper are:

1. The developed 1-D model can be used to accurately predict the NG-DI combustion process over a wide range of operating conditions with a fixed set of tuning parameters.
2. The 1-D model provides good accuracy for performance and cumulative emissions over a transient drive cycle.
3. The model can be used to estimate emissions penalties encountered during transient processes, particularly the NOx increase observed in a tip-out transient.

Future work is currently in progress to quantify the transient penalty share in different real-world drive cycles. Nevertheless, this study demonstrates the potential of the developed model to be used in evaluating engine performance and emission behavior when combined with a hybrid powertrain.

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