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Modeling and Simulation of Direct Injection Diesel Engine to Analyze Combustion and Emission using KIVA 3V Code

B V Krishnaiah [1]

Associate Professor, Department of Mechanical Engineering, Narayana Engineering College,Gudur SPSR Nellore District krishnaiahphd@gmail.com

Dr B Balu Naik [2]

Professor, Department of Mechanical Engineering JNT University Hyderabad Hyderabad banothbn@rediffmail.com

Abstract
Internal Combustion (IC) engines are complex systems having a multitude of parameters which interact with each other. The rapid development of computer technology has encouraged the use of complex simulation techniques to quantify the effect of the fundamental processes in the engine systems. In this paper a model for IC engine is developed and simulated. The primary objective of this work is to model the combustion and emission process. Suitable modeling is done to incorporate analysis of NOx and Soot emission as a result of combustion process. The proposed model is implemented using a modified KIVA 3 Code and the results of the simulation are presented.

Keywords: IC, Modeling, NOx, Soot, KIVA

1. INTRODUCTION

Modeling is the simple representation of complex real world problem. Almost all the real world phenomena are complex and can be simplified by taking some assumptions. It is desired to develop the simplest possible model that incorporates the major features of the phenomenon of interest. Many models have been developed by many researchers to solve the complex combustion process of diesel engines [1-5]. Due to extreme complexity of engine processes and our inadequate understanding at a fundamental level, most engine models are incomplete. Models are used for design purpose, for complete understanding of processes and to predict engine behavior over a wide range of operating condition.

The theoretical models used in the case of internal combustion engines can be classified into two main groups: thermodynamic models and fluid dynamic models. Thermodynamic models are mainly based on the first law of thermodynamics and are used to analyse the performance characteristics of engines. Pressure, temperature and other required properties are evaluated with respect to crank angle or time. The engine friction and heat transfer are taken into account using empirical equations obtained from experiments. These models are further classified into two groups namely single-zone models and multi-zone models. On the other hand, multi-zone models are also called computational fluid dynamics models. They are based on the numerical calculation of mass, momentum, energy and species conservation equations in either one, two or three dimensions to follow the propagation of flame or combustion front within the engine combustion chamber. Two zone model consists of one non burning zone which contains pure air and other zone consists of fuel and combustion products called burning zone. First law of thermodynamics and state equations are applied in each of the two zones to yield cylinder temperatures and cylinder pressure histories. Using the two zone combustion model the combustion parameters and the chemical equilibrium composition were determined. Multi-dimensional models need detail information of many phenomena and large computation time. Single zone model though simple does not account for heterogeneous character of diesel engine. Therefore, it is reasonable to choose a two zone model which is simple and required reasonable computer time.

The advances achieved by current automotive engines would have been impossible without the simulation models providing these insights [6,7].Lyn et al. [8] analyzed the effects of injection timing, injection velocity and fuelling rate on the delay period. An increase in speed at constant load increases the peak pressure and temperature, due to the decrease in heat transfer, resulting in a slight decrease in delay period as analysed by Wong et al. [9]. For engineering applications a semi-empirical relation based on chemical chain reactions called as Weibe‟s function is used to find heat release rate [10, 11]. However a single Weibe‟s function is not able to predict the heat release rate during early premixed burning. Thus a double Weibe‟s function is required for accurate prediction direct injection diesel engine [10, 12].

The combustion process in diesel engine is extremely complex due to transient and heterogeneous nature of combustion which is mainly controlled by turbulent mixing of fuel and air. High speed photography studies and in-cylinder sample collection have revealed some interesting characteristic of combustion phenomena [10]. Ignition delay in diesel engines has a direct effect on engine efficiency, noise and exhaust emissions. A number of parameters directly affect the ID period, among them cylinder pressure and temperature, swirl ratio and misfire. A number correlations use an Arrhenius expression similar to that proposed by Wolfer [13] in 1938 where he measured the ignition delay as a function of pressure and temperature. Watson [12] developed an ID correlation using a diesel engine under steady state conditions which is still widely used. Later Assanis et. al. [14] developed an ignition delay correlation for predicting the delay period in

a heavy-duty turbocharged direct injection diesel engine running under both steady state and transient operation.
The primary objective of the proposed work is to model and simulate the combustion and emission process in direct injection diesel engine. In this paper a direct injection diesel engine is modeled and simulated using modified KIVA 3 code. Wiebes combustion model is used for modeling the combustion. Similarly emission of NOx and Soot are also suitably modeled. The modeled features are incorporated in the form of a modified KIVA code and the results of the simulation are presented.

2. MODEL DESCRIPTION

During compression stroke, only one zone (of pure air) exists. Then, the first law of thermodynamics for a closed system is applied together with the perfect gas state equation (Heywood). The change in internal energy can be expressed as follows:

$$\frac{d(mu)}{d\theta} = \frac{dQr}{d\theta} - \frac{dQh}{d\theta} - \frac{dW}{d\theta} \quad (1)$$

By replacing the work transfer term $\frac{dW}{d\theta}$ with $P\frac{dV}{d\theta}$ or by the ideal gas law PV=mRT, the above equation (1) can be arranged as

$$\frac{d(mu)}{d\theta} = \frac{dQr}{d\theta} - \frac{dQh}{d\theta} - P\frac{dV}{d\theta} \quad (2)$$

Where, V is the instantaneous cylinder volume with respect to crank angle which is given by

$$V=V_{C1}+\left(\frac{\pi D^2}{4}\right)r[1+\lambda^{-1} - cos\emptyset - \sqrt{\lambda^{-1} - sin^2\emptyset}] \quad (3)$$

In the above equations, the term du is given as fourth order polynomial expressions of the absolute temperature T, including the enthalpy of formation at absolute zero. Internal energy calculation as a function of temperature:

$$hi/(RmolT)=ai1+ ai2\ T/2+ai3\ T2\ /3+ ai4\ T3/4+ai5\ T4/5+ai6/T \quad (4)$$
$$ui = hi - RT$$

For the surrounding air zone, which only loses mass (air) to the burning zone, the first law of thermodynamics for the unburned zone is written as

$$dE = dQ - pdV - hadma \quad (5)$$

The burning zone not only receives mass from the air zone, but also there is an enthalpy flow from the fuel which is ready to be burned in the time step. So, the first law of thermodynamics for the burning zone becomes

$$dE = dQ\text{-}pdV + hadma + hfdmf \quad (6)$$

The first law of thermodynamics for the combustion in time step dt is

$$f(E)=E(T2) - E(T1) - dQ + dW + dmf\ Qvs =0 \quad (7)$$

If f(E) is greater than the accuracy required new value of T2 is calculated using the Newton-Raphson numerical method. The unburned zone temperature is calculated using the equation.

$$T_u = T_{SOC}\left(\frac{P}{P_{SOC}}\right)(\gamma - 1)/\gamma \quad (8)$$

3. WIEBE'S COMBUTION MODEL

Wiebe function is used to predict the mass fraction burn and burn rate in internal combustion engines operating with different combustion systems and fuels [10]. Wiebe linked chain chemical reactions with the fuel reaction rate in internal combustion engines and his approach was based on the premise that a simple one-step rate equation will not be adequate to describe complex reacting systems such as those occurring in an internal combustion engine. Moreover, developing and solving rate equations which account for the simultaneous and sequential interdependent chain and chain branching reactions would be time consuming and tedious task. He argued that for engineering application the details of chemical kinetics of all the reactions could be bypassed and a general macroscopic reaction rate expression could be developed based on the concept of chain reactions.The Wiebe functions for the non-dimensional burn fraction x and its derivative w (burn rate) as functions of degrees crank angle can be written as

$$X=1\text{-}e^{-6.908(\emptyset/\emptyset d)^{m+1}} \quad (9)$$

$$W=\frac{dx}{d\emptyset}=\frac{6.908(m+1)}{\emptyset d}\left(\frac{\emptyset}{\emptyset d}\right)^m e^{-6.908(\emptyset/\emptyset d)^{m+1}} \quad (10)$$

or the non-dimensional burn fraction x and its derivative w (burn rate) as functions of time t can be written as

$$X=1\text{-}e^{-6.908(t/td)^{m+1}} \quad (11)$$

$$W=\frac{dx}{dt}=\frac{6.908(m+1)}{td}\left(\frac{t}{td}\right)^m e^{-6.908(t/td)^{m+1}} \quad (12)$$

The time it takes to reach maximum burn rate tm can be found by differentiating equation (12) and equating the result to zero

$$t_m=t_d\left(\frac{m}{60908(m+1)}\right)^{1/(m+1)} \quad (13)$$

The corresponding burn fraction is

$$X_m=1\text{-}\exp(-6.908(t_m/t_d)^{m+1}) \quad (14)$$

From above equations (11) and (12)

$$X_m=1\text{-}\exp(-m/(m+1))$$

Wiebe suggested the physical meaning of the exponent m which was based on equation (13), which shows that for a given combustion duration the time it takes for maximum burn rate to be reached is determined solely by the magnitude of m, which, in turn, determines the magnitude of the

maximum burn rate (equation (13)).When calculating the heat release, prior knowledge of actual overall equivalence ratio is necessary. The term equivalence ratio is defined as the ratio of actual air-fuel ratio to the stoichiometric air-fuel ratio. This helps in fixing the mass of fuel to be admitted.

4. EMISSION MODEL

In a combustion process, fuel and oxidizer react to produce products of different composition. The theory of combustion is a complex process and has been a topic of intensive research for many years. Let us represent the chemical formula of a fuel as $C\alpha H\beta O\gamma N\delta$.

Nitric oxide formation model

The current approach to modeling NOx emissions from diesel engines is to use the extended Zeldovich thermal NO mechanism and neglects other sources of NOx formation [15]. The extended Zeldovich mechanism consists of the following mechanisms

$O + N2 \longleftrightarrow NO + N$

$N + O2 \longleftrightarrow NO + O$

$N + OH \longleftrightarrow NO + H$

The change of NO concentration is expressed as follows:

$$\frac{d(NO)}{dt} = 2(1-\alpha^2)\frac{R1}{1+\alpha R1/(R2+R3)} \quad (15)$$

Where Ri is the one-way equilibrium rate for reaction i, defined as

$R1 = k_{1f}(N)_e(NO)_e$, $R2 = k_{2f}(N)_e(O2)_e$,

$R3 = k_{3f}(N)_e(OH)_e$, $\alpha = (NO)/(NO)_e$

Net Soot formation model

The exhaust of CI engines contains solid carbon soot particles that are generated in the fuel rich regions inside the cylinder during combustion. Soot particles are clusters of solid carbon spheres with HC and traces of other components absorbed on the surface. They are generated in the combustion chamber in the fuel rich zones where there is not enough oxygen to convert all carbon to CO2. Subsequently as turbulence motion continue to mix the components most of these carbon particles find sufficient oxygen to react and form CO2.Thus soot particles are formed and consumed simultaneously in the combustion chamber. The net soot formation rate was calculated by using semi-empirical model proposed by Hiroyasu et. al. (1983). According to this model the soot formation rate (index sf) and soot oxidation rate (index so) was given by

$$\frac{dm_{sf}}{dt} = A_{sf} dm_f^{0.8} p^{0.5} \exp\left(-\frac{E_{sf}}{R_{mol}T}\right) \quad (16)$$

$$\frac{dm_{so}}{dt} = ` A_{so} m_{sn} \left(\frac{p_{o_2}}{p}\right) p^n \exp\left(-\frac{E_{so}}{R_{mol}T}\right) \quad (17)$$

Where pressure are expressed in bar, dm_{sf} is the unburned fuel mass in kg to be burned in time step dt. Therefore the net soot formation rate is expressed as

$$\frac{dm_{sn}}{dt} = \frac{dm_{sf}}{dt} - \frac{dm_{so}}{dt} \quad (18)$$

5. KIVA 3V CODE

KIVA is a family of Fortran-based Computational Fluid Dynamics software developed by Los Alamos National Laboratory (LANL) [16]. The software predicts complex fuel and air flows as well as ignition, combustion, and pollutant-formation processes in engines. The KIVA models have been used to understand combustion chemistry processes, such as auto-ignition of fuels, and to optimize diesel engines for high efficiency and low emissions. The first public release of KIVA was made in 1985 through the National Energy Software Center (NESC) at Argonne National Laboratory, which served at the time as the official distribution hub for Department of Energy-sponsored software. Distribution of KIVA continued through the Energy Science and Technology Software Center (ESTSC) in Oak Ridge, Tennessee until 2008, when distribution of multiple versions of KIVA returned to LANL's Technology Transfer Division (TT)

KIVA, a transient, three-dimensional, multiphase, and multicomponent code for the analysis of chemically reacting flows with sprays has been under development at LANL for decades. The code uses an Arbitrary Lagrangian Eulerian (ALE) methodology on a staggered grid, and discretizes space using the finite volume method [16]. The code uses an implicit time-advancement with the exception of the advective terms that are cast in an explicit but second-order monotonicity-preserving manner. Also, the convection calculations can be subcycled in the

Although specifically designed for simulating internal combustion engines, the modularity of the code facilitates easy modifications for solving a variety of hydrodynamics problems involving chemical reactions. The versatility and range of features have made KIVA programs attractive to a variety of non-engine applications as well; these range from convection towers to modeling silicon dioxide condensation in high pressure oxidation chambers. Other applications have included the analysis of flows in automotive catalytic converters, power plant smokestack cleaning, and pyrolytic treatment of biomass, design of fire suppression systems, Pulsed Detonation Engines (PDEs), stationary burners, aerosol dispersion, and design of heating, ventilation, and air conditioning systems. The code has found a widespread application in the automotive industry.

KIVA-3V is the most mature version of KIVA still maintained and distributed through LANL KIVA-3V uses a block-structured mesh with connectivity defined through indirect addressing. The departure from a single rectangular structure in logical space allows complex geometries to be modeled with significantly greater efficiency because large regions of deactivated cells are no longer necessary. Cell-face boundary conditions permit greater flexibility and

simplification in the application of boundary conditions. KIVA-3V also contains a number of significant improvements over its predecessors. New features enhanced the robustness, efficiency, and usefulness of the overall program for engine modeling. Automatic restart of the cycle with a reduced time step in case of iteration limit or temperature overflow effectively reduced code crashes. A new option provided automatic deactivation of a port region when it is closed from the cylinder and reactivation when it communicates with the cylinder. Extensions to the particle-based liquid wall film model made the model more complete and a split injection option was also added. A new subroutine monitors the liquid and gaseous fuel phases and energy balance data and emissions are monitored and printed. In addition, new features were added to the LANL-developed grid generator, K3PREP, and the KIVA graphics post processor, K3POST.

6. RESULTS

A modified KIVA 3V code is used to simulate and analyze the performance of the proposed model. The specifications of the engine modeled are illustrated in the Table 1. The necessary modeling parameters are fed and modeled initially using K3PREP solved using the code and processed using K3POST.

Table 1.0: Engine specifications

Bore	13.716 cm
Stroke	16.51 cm
Length of Connecting Rod	26.3 cm
Squish	0.4221 cm
Compression Ratio (CR)	15:1
RPM	1600
Type of Fuel	$C_{14}H_{30}$

Similarly other factors that are considered in this model are listed in the Table (2.0). These parameters are vital for further analysis and modeling of combustion and emission.

Table 2.0: Factors Considered in Modeling of Combustion and Emission Process

Cylinder Wall Temperature	433.3K
Head Temperature	523.3K
Piston-Gas Side Surface Temperature	553.0K
Fuel Temperature at Injection	341.0K
Intake Surge Tank Pressure	1.96 e+6 dyn/cm^2
Intake Surge Tank Temperature	325.0K

The performance data for the simulated model is presented in the Table (3.0). The results are simulations of the modified KIVA 3V code to incorporate the specifications listed in Table (1.0) and Table (2.0)

Table (3.0): Performance metrics of the simulated model

Brake Mean Effective Pressure(bar)	9.589
Net Indicated Mean Effective Pressure(bar)	10.387
Gross Indicated Mean Effective Pressure(bar)	6.844
Friction Mean Effective Pressure(bar)	0.800
Brake Power(kW)	31.191
Friction Power(kW)	2.602
Net Indicated Power (KW)	33.793
BSFC (g/(kW-hr))	249.45
Fuel Flow Rate(lb/hr)	17.156

The loads acting on the crankshaft mainly derive from two different effects, the load due to variation of gas pressure in consequence of the combustion process and the ones related to the moving of inertial masses. Identifying the pressure and modeling inside a combustion chamber is very essential in identifying the force acting on the piston during the combustion cycle. The Figure 1 represents the variation in pressure inside the combustion chamber for the model simulated in this work. The variation is plotted against the movement in crank shaft represented using crank angle.

The variation of temperature inside the IC engine as function of crankshaft movement is presented in the Figure 2. The model is capable of predicting the variation in temperature inside the combustion chamber through the process of ignition and combustion.

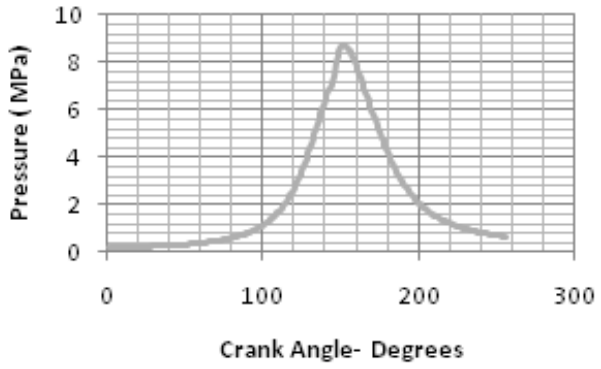

Figure (1): Variation of cylinder pressure as function of crank angle

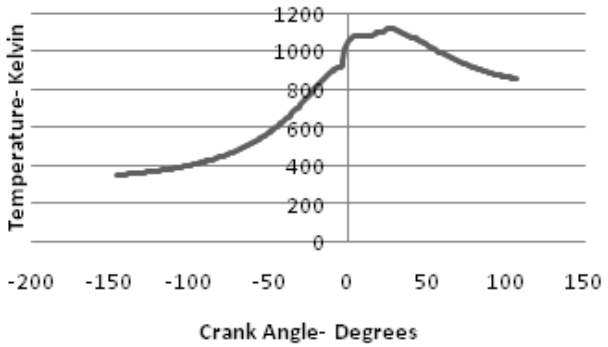

Figure (2): Variation of Temperature inside combustion chamber.

The simulated model is capable of capturing the changes in the cylinder volume during the combustion cycle. The figure 3 illustrates the change in volume of the cylinder as a function of crank angle.

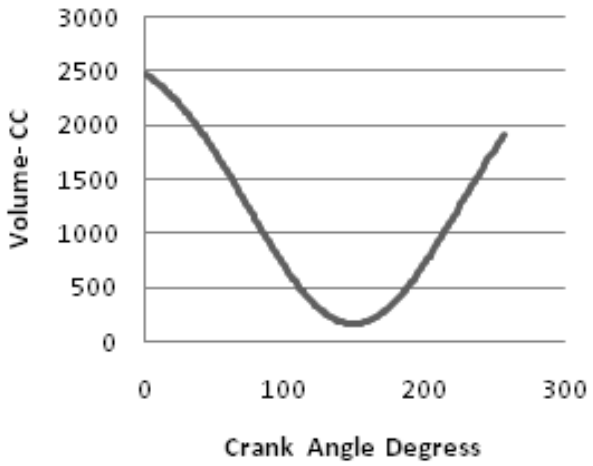

Figure (3): Change in cylinder volume during combustion process

The proposed model and the modified KIVA code are also capable of capturing the turbulence experienced in the combustion chamber. The KIVA code provides the necessary turbulence analysis. The Turbulent Kinetic Energy (TKE) of the flow indicates its strength as a whole. Figure 4 shows the variation of the TKE with crank angle during the combustion cycle. The turbulence controls the rate of flow dissipation, heat transfer and the rate of flame propagation and it is quantified by TKE within the cylinder.

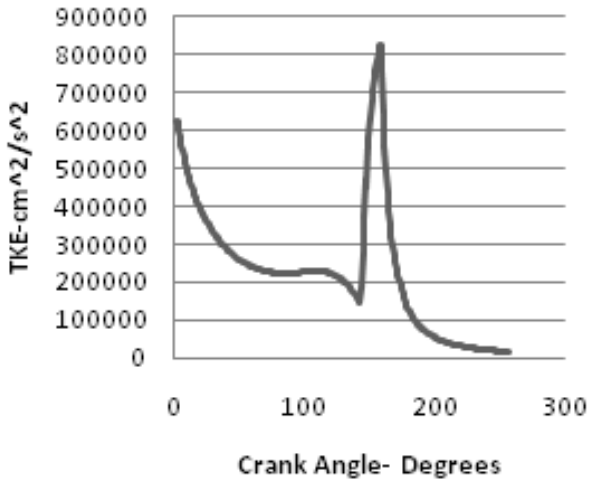

Figure (4): Total kinetic energy as a function of crank angle

Similarly the figure 5 presents the plot of turbulence dissipation rate as a function of crankshaft angle.

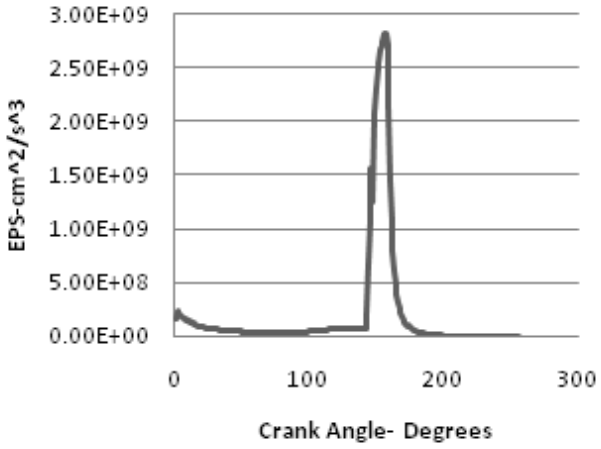

Figure (5): Plot of turbulence dissipation rate

In diesel engine exhaust, NOx is predominantly composed of NO, with lesser amounts of NO2. Other oxides of nitrogen, such as N2O, N2O5, and NO3 are negligible. In general, NOx formation mechanisms are described as thermal NOx, prompt NOx and fuel NOx. Under most diesel engine combustion conditions, thermal NOx is believed to be the predominant contributor to total NOx. At high temperatures, occurring within the combustion chamber of a diesel engine, N2 and O2 can react through a series of chemical steps known as the Zeldovich mechanism. The rate of formation of NOx increases rapidly with increasing temperature. The figure illustrates the plot the production of NOx against changes in crank angle.

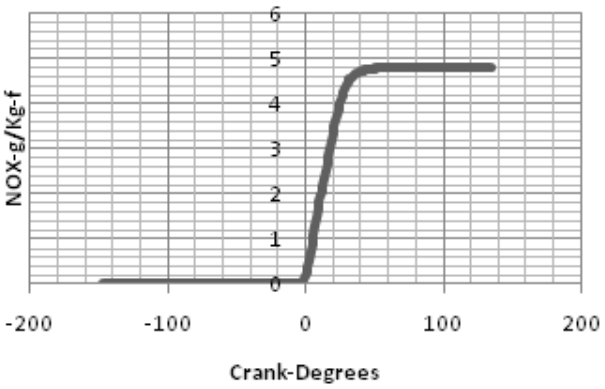

Figure (6): Quantification of NOx formation

Similarly the figure depicts the formation of soot as a function as there is variation in crank angle, which can be correlated with occurrence of ignition

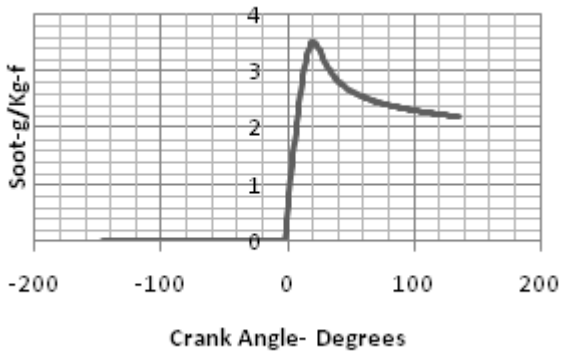

Figure (7): Quantification of Soot formation

The proposed model and the simulation methodology are capable of performing all the necessary analysis for studying the combustion process and emission process for a direct injection diesel engine.

7. CONCLUSION

Diesel engines, particularly direct injection types, have been an important choice as prime movers in heavy-duty applications such as on-road, off-road, marine and industrial usage due to their high brake thermal efficiency. In this paper the results of simulation for a direct ignition has been presented. The results of simulation show the suitability of the model and that of modified code in analyzing different aspects of combustion in an IC engine. The proposed approach is also capable of analyzing emission and turbulence. This model enhances the opportunities to study the performance of diesel engine under different scenarios.

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