Simplified Analysis of Pulse Detonation Rocket Engine Blowdown Gasdynamics and Performance

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Pulse detonation rocket engines (PDREs) offer potential performance improvements over conventional designs, but represent a challenging modeling task. A simplified model for an idealized, straight-tube, single-shot PDRE blowdown process and thrust determination is described and implemented. In order to form an assessment of the accuracy of the model, the flowfield time history is compared to experimental data from Stanford University. Parametric studies of the effect of mixture stoichiometry, initial fill temperature, and blowdown pressure ratio on the performance of a PDRE are performed using the model. PDRE performance is also compared with a conventional steady-state rocket engine over a range of pressure ratios using similar gasdynamic assumptions.

Introduction

PULSED detonation rocket engines (PDREs) have generated considerable research interest in recent years as a chemical propulsion system potentially offering improved performance and reduced complexity compared to conventional rocket engines. The detonative mode of combustion employed by these devices offers a thermodynamic advantage over the constant-pressure deflagrative combustion mode used in conventional rocket engines and gas turbines. However, while this theoretical advantage has spurred a great deal of interest in building PDRE devices, the unsteady blowdown process intrinsic to the PDRE has made realistic estimates of the actual propulsive performance problematic. The recent review article by Kailasanath highlights some of the difficulties in comparing the available experimental measurements with numerical models.

The goal of this paper is to improve understanding of PDRE blowdown gasdynamics and performance issues through use of a simplified model that captures the essential features of the unsteady blowdown process, and yet remains computationally inexpensive. The details of the model are provided first in order to form an appreciation for the assumptions and simplifications imposed. The model is compared to experimental data from Stanford University in order to assess the accuracy of the calculations. Parametric studies of the effect of mixture stoichiometry, fill temperature, and blowdown pressure ratio on performance are reported. A comparison of the performance of an idealized straight-tube PDRE with a conventional steady-state rocket engine (SSRE) is also provided.

Theoretical Model

The PDRE system studied here is highly idealized, consisting of a constant-area detonation tube with one end closed and the other end open to the environment. The tube is pre-filled with a gaseous propellant mixture with no initial velocity or outflow to the environment - an idealization that could be approximated in practice by covering the open end of the detonation tube with a thin plastic diaphragm. The detonation is initiated instantaneously at the closed end of the device. No nozzle is fitted to the end of the tube. As this level of analysis, the specific impulse per charge of fuel is independent of the length of the tube.

The Chapman-Jouguet (C-J) post-detonation gas conditions are calculated using the CET89 version of the NASA thermochemical code. The J-D, unsteady method of characteristics is used to calculate the flowfield following the detonation front. See the compressible flow texts by Zuckrow and Hoffman and Thompson for details of this method. The gas composition is presumed to remain frozen throughout the blowdown period, and the ratio of specific heats, , is fixed at the value provided by the C-J detonation calculation.

An earlier version of this code explicitly modeled two rarefaction waves in the blowdown process. The first rarefaction wave immediately follows the detonation front as it travels down the length of the tube. This wave is necessary to reduce the gas velocity induced by the detonation wave so that it matches the zero-velocity wall boundary condition at the closed end of the tube. The second rarefaction wave is initiated when the detonation front reaches the end of the tube and exits to the ambient environment. The detonation is presumed to dissipate rapidly in the ambient environment, and is effectively ignored after reaching the exit. In the earlier model, the second rarefaction was modeled as a centered expansion wave radiating from the tube exit point, and the interaction processes with both the first rarefaction, and the closed head end of the tube were

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explicitly calculated. While this approach was extremely
inexpensive computationally, there is a question as to how
well this models the true exit boundary condition of a deto-
nation tube. A centered expansion is only appropriate for a
truly 1-D exit flow scenario, and any real PDRE device will
of course be multidimensional. The work of Kailasanath
shows the critical effect of the exit boundary condition on
the flow history, and thus performance, particularly at
longer timescales.

In the current model, the detonation front and first rar-
efaction fan are modeled explicitly as before. However,
once the detonation reaches the exit of the tube, the sub-
sequent flowfield is calculated using unit processes for 1-
D, unsteady flow at grid points spaced every 2 mm in the
tube. This approach adds some computational expense,
but allows much greater flexibility in modeling the exit
flow boundary condition. For the purposes of this work, a
constant-pressure \( P_{\text{exit}} = P_{\text{ambient}} \) exit boundary condition is
used. Typical tube lengths are 1.0 m (501 grid points) for
the parametric studies reported later in this paper. The
approach also remains computationally inexpensive. Program
execution times typically ranged from 10-30 seconds.

The time-dependent thrust in this model is calculated
from the difference between the instantaneous closed end
wall pressure and the ambient pressure. The thrust is in-
tegrated in time until the point when the closed wall pressure
equals the ambient value, i.e. the thrust drops to zero. Thus,
this thrust calculation represents the theoretical maximum
impulse that can be delivered per charge of fuel, given
the assumptions of the model. An example thrust history
for a stoichiometric H\(_2\)-O\(_2\) mixture at a fill temperature of
300 K, fill pressure of 1 Atm, and an ambient pressure of
1 Atm, is shown in Fig. 1. The blowdown can essentially be
thought of as occurring in three phases. In the first phase,
the detonation is initiated and travels down the length of the
tube. The length of this phase in time is
\[ \tau_1 = \frac{L_{\text{tube}}}{C_{\text{D}-1}} \]
where \( L_{\text{tube}} \) is the length of the tube, and \( C_{\text{D}-1} \) is the C-
J detonation velocity. In the second phase, the head of
the rarefaction wave initiated at the exit interacts with the
right-running expansion following the detonation, and then
travels back up the tube in order to communicate the exit
boundary condition to the remainder of the gas in the tube.
The length of this phase is approximately
\[ \tau_2 \sim \frac{L_{\text{tube}}}{c_3} \]
where \( c_3 \) is the sound speed of the quiescent combustion
products after being slowed by the right-running rarefaction
wave. The third phase is comprised of the complex
wave interactions that are initiated when the exit expansion
wave interacts with the closed end wall. The length of this
phase is strongly dependent on the blowdown pressure ra-
tio.

Comparison of Model with Experimental
Data

The current model is compared with experimental results
from Stanford University\(^8\) in Fig. 2. The experimental re-
results were obtained from a detonation tube 1.6 m in length,
and using stoichiometric C\(_2\)H\(_4\)-O\(_2\) (at \( T_{\text{ini}} = 298 \) K and
\( P_{\text{ini}} = 1 \) Atm) as the propellant mixture. The measure-
ments were acquired at a location 1.44 m from the head
(closed) end of the tube. The model ran this case using a
point spacing of 2 mm (801 grid points).

There is generally good agreement between the exper-
imental measurements and the flowfield history calculated
by the model. There is a consistent overprediction of
both the pressure (by 1-2 Atm) and the temperature (by
500-600 K) at longer flow times (from roughly 800 \( \mu \)s after
detonation arrival). It is reasonable to expect that the con-
stant-\( \gamma \), frozen chemistry, and 1-D isentropic flow as-
sumptions in the model will have a considerable impact on
the results at these times. Additionally, no heat transfer to
the tube is assumed in the model. The velocity calculations
show good agreement to within roughly 150 m/s, and often
much closer, until approximately 3800 \( \mu \)s. After that point
the model and measurements diverge more substantially.
Given the proximity of the measurement station to the exit
of the tube, and the relatively low remaining gas pressure
(1-2 Atm) present in the tube at that point, this discrep-
ancy is likely due to the exit flow boundary condition.

In general the model captures the qualitative behavior
of the experimental measurements quite well. Addition-
ally, the performance figures calculated by the model are
in good agreement with those reported previously. Kailas-
anth\(^7\) reviewed experimental performance measurements
from the literature, and reports estimates for stoichiometric
C\(_2\)H\(_4\)-O\(_2\) specific impulse as 162-165 s, and volume-based
total impulse as roughly 2100 N-s/m\(^3\). These estimates are
within roughly 5% of the values calculated by the model
(175.4 s, 2180 N-2/m\(^3\) respectively) for this mixture.

Parametric Study Results

The model was used to perform parametric studies of
the effect of mixture stoichiometry, fill temperature, and
blowdown pressure ratio on the performance of an ideal-
ized, straight-tube PDRE. The charge-based, single-shot
total impulse, specific impulse and blowdown time were
all determined using the model. Additionally, the perfor-
mance of an idealized, straight-tube PDRE is compared
with a conventional steady-steady rocket engine.

Effect of Stoichiometry on Performance

The charge-based specific impulse for hydrogen, as well
as several hydrocarbon fuels, as a function of mixture sto-
ichiometry is shown in Fig. 3. In all cases studied here
the initial temperature of the mixtures was 300 K and the
initial pressure was 1 Atm. Although the parametric im-
pact of blowdown pressure ratio is studied more completely
in a later section of this paper, results are plotted for fi-
nal blowdown pressures of both 1 Atm and 0.01 Atm. In
each case the final pressure is also equal to the ambient
pressure outside the tube. Note that the H\(_2\)-O\(_2\) system
exhibits consistently higher specific impulse, compared to
all the hydrocarbons, throughout the range of stoicho-
metries studied. All of the mixtures exhibit at least some
benefit in specific impulse by operating fuel-rich. The
peak specific impulse for the H₂-O₂ system is achieved at very fuel rich conditions, a stoichiometric ratio of approximately 2.8 for blowdown to 1 Atm, and 3.8 for blowdown to 0.01 Atm. The optimum point for the hydrocarbons is typically achieved at a lower ratio. The hydrocarbon fuels exhibit higher total impulse delivered per charge, and longer blowdown times per charge, than the H₂-O₂ system. In general, the heavier hydrocarbons exhibit larger total impulse and longer blowdown times.

Effect of Fill Temperature on Performance

The effect of the initial fill temperature on the specific impulse of the various propellant mixtures is shown in Fig. 4. Investigation of this parameter is especially relevant since an operational boost-class or upper-stage PDRE would likely operate with cryogenic storage of at least some of the propellants. In all cases: studied here, the mixture stoichiometry was 1.0 and the initial pressure was 1 Atm. As was done in the stoichiometry study, complete results were generated for two different final blowdown pressures: 1 Atm and 0.01 Atm. Initial temperatures were varied from 300 K to 180 K. Reviewing the 1 Atm blowdown cases first, we find that the initial temperature has a clear impact on performance. Specific impulse for the H₂-O₂ system increases by 11% over the temperature range, while the specific impulse for the hydrocarbon-O₂ mixtures increases by 7–8%. The total impulse delivered per charge increases by 86% for hydrogen, and roughly 78–80% for the hydrocarbons. There is a modest increase in blowdown time for all mixtures. Reducing the initial temperature from 300 K to 180 K results in a 67% increase in the density of the gas mixture, assuming the same initial pressure. Therefore, there must be an additional factor that results in increased thrust per charge as the temperature is reduced. That factor is the increase in the Mach number of the C-J detonation as the initial temperature is reduced, from a value of \( M_{C-J} = 5.26 \) at 300 K to \( M_{C-J} = 6.83 \) at 180 K for H₂-O₂. The pressure jump across a shock or detonation wave is a very strong function of the Mach number, in this case resulting in a nearly 76% increase in the post detonation pressure. This increase in pressure contributes directly to the increased total impulse by providing both a larger peak thrust level (during \( \tau_1 \) and \( \tau_2 \)), as well as a longer blowdown period to the ambient condition (\( \tau_3 \)).

The results for blowdown to 0.01 Atm are also illuminating. There is effectively no change in hydrocarbon-O₂ mixture specific impulse, while there is an actual slight decrease in H₂-O₂ specific impulse. This is primarily due to the fact that the performance of rocket-type engines is much more strongly sensitive to changes in pressure at lower pressure ratios than at high pressure ratios. This effect is explained in greater detail in the next section.

Effect of Blowdown Pressure Ratio on Performance

The blowdown pressure ratio is one of the most critical parameters affecting PDRE performance. The blowdown ratio is defined here as the ratio of the initial fill pressure of the tube to the ambient pressure outside the tube. Note again that the model is run until the pressure at the closed end of the tube equals the ambient pressure and the thrust vanishes. Therefore, for a given initial fill pressure, we would expect that reducing the ambient pressure (hence increasing the blowdown pressure ratio) would result in additional thrust delivered per charge. Additionally, we would expect the blowdown time to increase as well. The plot in Fig. 5 shows the effect of blowdown pressure ratio on the charge-based, single-shot specific impulse for stoichiometric H₂-O₂ as well as several hydrocarbon-O₂ mixtures. Two sets of calculations are shown for each fuel: one at an initial pressure of 1 Atm, and another at 10 Atm. In all cases studied here the initial temperature of the mixtures is 300 K. As expected, the H₂-O₂ system exhibits a consistently better specific impulse across the range of blowdown ratios studied. The hydrocarbon-O₂ mixtures consistently exhibit higher total impulse per charge, and longer blowdown times per charge, and both factors tend to scale with the molecular weight (and thus overall density) of the fuel. The impulse for one charge increases by approximately 34% for H₂-O₂ (18–22% for the hydrocarbon-O₂ mixtures) as the blowdown pressure ratio is increased from 1 to 10. There is diminishing improvement at higher pressure ratios: only 3–5% when the blowdown pressure ratio is increased from 10 to 100, and very marginal gain beyond that point. The blowdown time also increases steadily as a function of pressure ratio. The results for initial pressures of 10 Atm show slightly higher specific impulse due to the shift in thermodynamic equilibrium at higher pressures.

These results clearly show the tradeoff between obtaining the maximum thrust per charge of fuel-oxidizer mixture by allowing the tube to blow down to lower pressures, and the competing interest of the increase in blowdown time required to accomplish this. The increase in blowdown time limits the rate at which a cyclic device could operate, and thus limits the time-averaged thrust capability. Examination of the example thrust history profile shown in Fig. 1 clearly shows the diminishing returns of thrust at longer timescales. It is fair to point out that the blowdown times are fairly sensitive to the exact boundary conditions used, and that the constant ambient pressure condition used here is relatively conservative. As shown by Kailasanath, exit boundary schemes which allow for a gradual decay in pressure to the ambient value can significantly increase the blowdown time.

The specific impulse of a single-shot, straight-tube PDRE is compared with the performance of a conventional steady-state rocket engine for the H₂-O₂ system in Fig. 6. The SSRE performance is calculated assuming the same initial conditions as the PDRE fill mixture, constant pressure combustion, and expansion through a nozzle assuming constant-\( y \), as is the case in the PDRE model. Two rocket curves are shown in the figure: one curve assumes a sonic nozzle, and the other assumes that an optimized supersonic nozzle is fitted to the rocket at each pressure ratio. As there is no nozzle in our model, the comparison of the straight-tube PDRE with a sonic nozzle SSRE is perhaps the most
appropriate. The plot shows the large performance advantage a PDRE enjoys over either type of conventional rocket engine at lower blowdown pressure ratios. This advantage is greatest when the ambient pressure matches the initial pressure (blowdown ratio of 1), since a conventional SSRE will produce no thrust at this condition. The PDRE maintains this advantage until the blowdown ratio reaches roughly 7 (using these relatively simple models). At higher blowdown pressure ratios, the PDRE maintains a significant lead over a SSRE with a sonic nozzle, but is outperformed by a SSRE with an optimized supersonic nozzle. This is a result of the relatively large internal energy remaining in portions of the PDRE exhaust time history. These studies clearly point out the large advantage PDREs enjoy for low pressure ratio applications. In any environment with a large ambient pressure, the self-pressurization capability of the PDRE presents compelling advantages. Additionally, the results show that there is a critical need for further research in PDRE nozzle designs if the ultimate performance potential of these devices is to be realized for high-altitude and high-thrust applications.

Summary

A simplified model for an idealized, straight-tube, single-shot PDRE blowdown process and thrust determination has been described and implemented. The model shows generally good agreement with experimental measurements from the literature. Parametric studies of the effect of mixture stoichiometry, initial fill temperature, and blowdown pressure ratio on the performance of a PDRE have been performed using the model. These studies point to avenues for performance enhancement within certain regimes. Additionally, PDRE performance has also been compared with a conventional SSRE over a range of pressure ratios using similar gasdynamic assumptions. The comparison shows the distinct advantage PDREs offer for low pressure ratio applications, but point out the critical need for PDRE nozzle research for high-altitude and high-thrust applications.

Acknowledgements

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References:

5Thompson, P. A., Compressible-Fluid Dynamics, Department of Mechanical Engineering, Rensselaer Polytechnic Institute, 1988.
Fig. 1 Example thrust history calculated for an idealized, straight-tube PDRE. Propellant mixture: stoichiometric H₂-O₂. Test conditions: \( P_{\text{ini}} = 1.0 \text{ Atm} \), \( T_{\text{ini}} = 300 \text{ K} \), \( L_{\text{tube}} = 1.0 \text{ m} \).
Fig. 2  Comparison of model with experimental data from Stanford University. a) Pressure history, b) Temperature history, c) Velocity history. Propellant mixture: stoichiometric $\text{C}_2\text{H}_4\text{-O}_2$. Test conditions: $p_{\text{ini}} = 1.0 \text{ Atm}$, $T_{\text{ini}} = 298 \text{ K}$, $L_{\text{tube}} = 1.6 \text{ m}$, $L_{\text{meas}} = 1.44 \text{ m}$ (from head end).
Fig. 3  Effect of propellant mixture stoichiometry on performance characteristics. Test conditions: \( P_{\text{in}} = 1.0 \text{ Atm}, T_{\text{in}} = 300 \text{ K}, L_{\text{tube}} = 1.0 \text{ m}. \)
Fig. 4 Effect of initial propellant mixture temperature on performance characteristics. Test conditions: $P_{ini} = 1.0 \text{ Atm, } \phi = 1.0$, $L_{tube} = 1.0 \text{ m.}$
Fig. 5  Effect of blowdown pressure ratio on performance characteristics. Test conditions: $T_{in} = 300$ K, $\phi = 1.0$, $L_{tube} = 1.0$ m.
Fig. 6  Performance comparison of the idealized, straight-tube PDRE with a conventional steady-state rocket engine equipped with both sonic and variable-area, optimized supersonic nozzles. The specific heat ratio, \( \gamma \), is held constant in all models. Representative values of the nozzle expansion ratio, \( \varepsilon \), are shown on the supersonic nozzle curve. Propellant mixture: stoichiometric \( \text{H}_2\text{-O}_2 \). Test conditions: \( P_{\text{in}} = 10.0 \text{ A tm}, T_{\text{in}} = 300 \text{ K} \).
Performance Analysis of PDRE

Steady-State Rocket Engine
- Variable-area nozzle
- Combustion products
- Steady, variable-area flow

Pulsed Detonation Rocket Engine
- C-J detonation
- Combustion products
- Rarefaction waves (right running)
- Initial propellant mixture
- Unsteady, 1-D flow

- Pulsed Detonation Rocket Engines (PDREs) are a novel chemical propulsion concept which have been studied over the past several years.
- Performance claims of PDREs are based on thermodynamic advantage of detonative combustion, but typically ignore the unsteady blowdown process inherent to these devices.
- PRC is engaged in a fundamental study of PDRE gasdynamics to improve understanding of performance issues.
Simplified PDRE Cycle

1) Detonation initiation:
   - $U=0$
   - $P=P_i$

2) Combustion products:
   - C-J detonation
   - Rarefaction waves (right running)

3) Outflow:
   - Rarefaction waves (left running)

4) Rarefaction waves (left running)
   - Outflow

5) Combustion products at ambient pressure:
   - $U=0$
   - $P=P_o$

6) Injection of fresh propellant mixture

How do we Determine the Thrust?

Momentum Equation

$$F_{ix} + F_{bx} = \frac{d}{dt} \int_{CV} \rho \ u \ dV + \int_{CS} \rho \ u \ V \cdot dA$$

$$F_{sx} = \rho \ u^2 \ A + A (P_{ex} - P_{amb})$$

Steady-flow Rocket Engine

Pulsed Detonation Rocket Engine
How do we Determine the Thrust?

Momentum Equation

\[ F_{\text{x}} + F_{\text{BX}} = \frac{d}{dt} \int_{CV} \rho u \, dV + \int_{CS} \rho u \vec{V} \, dA \]

\[ F_{\text{SX}} = \int_{CS} (P_{\text{int}} - P_{\text{amb}}) \, dA \]

Steady-flow Rocket Engine

\[ F_{\text{SX}} = A (P_{\text{cl}} - P_{\text{amb}}) \]

Pulsed Detonation Rocket Engine

X-T Wave Diagram of PDRE Blowdown

- X-T Diagram shows time evolution of 1-D, unsteady flows
Typical PDRE Thrust History

$H_2O_2$, $\Phi = 1$, $T_{ini} = 300$ K, $P_{ini} = 1$ Atm, $P_{amb} = 1$ Atm

- PDRE thrust history can be visualized in three phases

MOC Parametric Study

- Utilized CET89 to calculate C-J detonation properties, and the method of characteristics to model the flow after the detonation
- Detonation initiation is assumed instantaneous
- Specific heat ratio, gamma, is constant throughout the blowdown
- Studied four possible PDRE fuels: $H_2$, $C_2H_2$, $C_2H_4$, $C_3H_8$
- Results characterized in terms of:
  - Thrust (Total Impulse)
  - Specific Impulse
  - Blowdown Time
- Studied impact of:
  - Mixture Stoichiometry
  - Initial Fill Temperature
  - Blowdown Pressure Ratio
Effect of Stoichiometry on Total Impulse

\[ T_{\text{ini}} = 300 \text{ K}, \ P_{\text{ini}} = 1 \text{ Atm}, \ P_{\text{amb}} = 1 \text{ Atm} \]

- HC Fuels generate increased thrust compared to \( \text{H}_2 \)
- Effect of stoichiometry on thrust is fuel-dependent

Effect of Stoichiometry on Blowdown Time

\[ T_{\text{ini}} = 300 \text{ K}, \ P_{\text{ini}} = 1 \text{ Atm}, \ P_{\text{amb}} = 1 \text{ Atm} \]

- Blowdown time for HC Fuels is longer than \( \text{H}_2 \)
- Effect of stoichiometry on blowdown time is fuel-dependent
Effect of Stoichiometry on Specific Impulse

\( \gamma_{\text{ini}} = 300 \, \text{K}, \, P_{\text{ini}} = 1 \, \text{Atm}, \, P_{\text{amb}} = 1 \, \text{Atm} \)

- \( \phi \) exhibits higher specific impulse than HC fuels
- Specific impulse peaks at \( \phi > 1 \)

Effect of Initial Fill Temperature on Total Impulse

\( \phi = 1, \, P_{\text{ini}} = 1 \, \text{Atm}, \, P_{\text{amb}} = 1 \, \text{Atm} \)

- Reductions in fill temperature result in higher charge density and thrust
Effect of Initial Fill Temperature on Blowdown Time

$H_2-O_2, \phi = 1, P_{ini} = 1 \text{ Atm}, P_{amb} = 1 \text{ Atm}$

- Reductions in fill temperature increase the blowtime time

Effect of Initial Fill Temperature on Specific Impulse

$H_2-O_2, \phi = 1, P_{ini} = 1 \text{ Atm}, P_{amb} = 1 \text{ Atm}$

- Specific impulse increases by 11% for $H_2-O_2$ as $T_{ini}$ decreases from 300 K to 180 K
**Effect of Blowdown Pressure Ratio on Specific Impulse**

- Specific impulse ranges from 175-190 when $Pr = 1$
- Increases to 205-250 at $Pr = 10$, and 210-260 at $Pr = 100$
- Marginal gains only after $Pr = 100$

**Effect of Blowdown Pressure Ratio on Blowdown Time**

- Blowdown time increases steadily at higher blowdown pressure ratios
Comparison of PDRE and SSRE

$H_2-O_2$, $\phi = 1$, $T_{ini} = 300$ K, $P_{ini} = 10$ Atm

![Graph showing performance comparison between PDRE and SSRE](image)

- PDRE has performance advantage at lower pressure ratios
- SSRE has performance advantage at higher pressure ratios

PDRE Performance Study - Conclusions

- A simplified PDRE gasdynamic blowdown and performance code has been developed based on the method of characteristics.
- Parametric studies of mixture stoichiometry, fill temperature, and blowdown pressure ratio have been conducted.
- There is a tradeoff between specific impulse and time-averaged thrust level in PDREs that is not present in conventional rocket engines.
- The idealized, straight-tube, PDRE has a performance advantage over any conventional SSRE at low blowdown pressure ratios ($P_{ini}/P_{amb} < 7$).
- At higher blowdown pressure ratios, the idealized PDRE maintains a performance advantage over a conventional SSRE with a sonic nozzle, but has inferior performance to a rocket with an optimized, variable-area supersonic nozzle.
- A clear need for nozzle research exists for PDREs.
- Comparisons of the MOC model with other analyses, numerical models, and experimental data are underway.
Numerical Modeling of Idealized PDRE

- Fluid (Euler) convection:
  - 2nd-order accurate (time and space) Harten-Yee symmetric-TVD algorithm (Yee, 1989)
  - Employs Roe's approximate Riemann solver modified for nonequilibrium ideal gases (Grossman and CInella, 1990) and modified to ensure species positivity (Larrouturou, 1991)

- Chemistry integration:
  - $\text{H}_2\text{O}_2$ reaction mechanism: 9 species, 18 reactions (Petersen et al, 1997)
  - Employs implicit trapezoidal method (uses Jacobian of source terms)
  - 1st-order timestep splitting between fluid and chemistry routines

Comparison of 1-D CFD and MOC Results

$\text{H}_2\text{O}_2$, $\phi = 1$, $T_{\text{ini}} = 280$ K, $P_{\text{ini}} = 1$ Atm, $P_{\text{amb}} = 1$ Atm

- Good agreement between 1-D CFD and MOC calculations
- Effect of detonation initiation conditions evident in CFD results
Comparison of MOC Results with Stanford Experimental Data

\[ \text{C}_2\text{H}_4\text{-O}_2, \phi = 1, T_{\text{ini}} = 298 \text{ K}, P_{\text{ini}} = 1 \text{ Atm}, P_{\text{amb}} = 1 \text{ Atm} \]

- Model captures essential features of SU measurements
- Model overpredicts pressure at longer times

\[ L_{\text{tube}} = 1.60 \text{ m} \]
\[ L_{\text{meas}} = 1.44 \text{ m} \]
(from head end)

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Comparison of MOC Results with Stanford Experimental Data

\[ \text{C}_2\text{H}_4\text{-O}_2, \phi = 1, T_{\text{ini}} = 298 \text{ K}, P_{\text{ini}} = 1 \text{ Atm}, P_{\text{amb}} = 1 \text{ Atm} \]

- Model captures essential features of SU measurements
- Constant-gamma assumption in model overpredicts temperature

\[ L_{\text{tube}} = 1.60 \text{ m} \]
\[ L_{\text{meas}} = 1.44 \text{ m} \]
(from head end)
Comparison of MOC Results with Stanford Experimental Data

$C_2H_4 - O_2, \phi = 1, T_{ini} = 298 \text{ K}, P_{ini} = 1 \text{ Atm}, P_{amb} = 1 \text{ Atm}$

- Generally good agreement between model and SU measurements
- Divergence at long flow times likely results from exit flow BC