

# QUASI-ONE DIMENSIONAL FLOW THROUGH A NOZZLE WITH A SHOCK

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# OVERVIEW



## University of California, Irvine

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## Masters Thesis

Mechanical and Aerospace Engineering, Fluid  
Mechanics



**Wanted something related to  
rocket engines**

# INTRODUCTION

- Van der Waal's Equation of State (EoS) 1873

$$P = \frac{RT}{v - b} - \frac{a}{v^2} \quad 1 = \frac{P}{\rho RT}$$

- Compressibility Factor - Z

$$Z = \frac{P}{\rho RT}$$

- Redlich-Kwong (1949)

$$P = \frac{RT}{v - b} - \frac{a/T^{0.5}}{v(v + b)}$$

- Soave-Redlich-Kwong (1971)

$$P = \frac{RT}{v - b} - \frac{a(T)}{v(v + b)}$$

# WHY USE SOAVE-REDLICH-KWONG



**Mainly Algebraic**



**Minimal Information Needed**

Specific Heat Capacity  
Critical Pressure  
Critical Temperature  
Acentric Factor  
Molecular Weight



**Addresses temperature and pressure variation**



**Addresses difference of species**

# PREVIOUS WORKS

- Johannes Diderik van der Waals (1873)
  - Equation everyone knows
- Redlich-Kwong (1949)
  - Shell Development Company
  - Identified new way of approaching temperature dependency
- Soave (1971)
  - Modified Redlich-Kwong
  - Equations used in this study
- Peng Robinson (1976)
  - Another EoS, often compared to Soave-Redlich-Kwong
- Various Works
  - Improvement of binary interaction coefficients
- Huron and Vidal (1979)
  - Defined new mixing rules for gases with multiple species
- Sirignano (2018)
  - Approximate Solution

# APPLICATIONS

- Originally developed by Shell company for fracking
- Vapor Equilibrium Studies
- Boilers Design
- Power Cycles
- Wind Tunnel Predictions
- Turbomachinery
- Working Fluids
- Hydraulics
- Shock Waves
- Compressible Flow
- Nozzle Design

# SCOPE



## Range of properties

Pressure: 10, 30, 50, 100, 200, 500 bar  
Temperature: 500, 1000, 2000, 4000 K



## Investigating value mores associated with rocket nozzle flow



## Some temperature dependent terms not modeled

Eg.

- Specific heat capacities
- Binary interaction coefficients

# ISENTROPIC FLOW

- Need to solve cubic EoS

$$Z = \frac{P}{\rho RT}$$

$$Z^3 - Z^2 + (A - B - B^2)Z - AB = 0$$

- Roots function takes a lot of computational time
- Used Cardano's Method for direct and more efficient calculations



# ISENTROPIC FLOW

- Normalized pressure and temperature by stagnation values
- Find A and B

$$\begin{aligned}
 P &= \frac{T_d}{T_0} \\
 T &= \frac{T_d}{T_0} \\
 A &= \frac{aP_d}{(R_u T_d)^2} = \frac{\hat{a}P}{T^2} \quad \hat{a} = \frac{aP_0}{(R_u T_0)^2} = \sum_{i=1}^N \sum_{j=1}^N \sqrt{\hat{a}_i \hat{a}_j} (1 - k_{ij}) X_i X_j \longrightarrow \hat{a}_i = \frac{aP_d}{(R_u T_d)^2} = 0.42748 \frac{T_{ci}^2}{P_{ci}} [1 + S_i (1 - \sqrt{\frac{T}{T_{ci}}})]^2 \\
 &\quad \longrightarrow T_{ci} = \frac{T_{ci,d}}{T_0} \\
 &\quad \longrightarrow P_{ci} = \frac{P_{ci,d}}{P_0} \\
 &\quad \longrightarrow S_i = 0.48508 + 1.5517\omega_i - 0.15613\omega_i^2 \\
 B &= \frac{bP_d}{R_u T_d} = \frac{\hat{b}P}{T} \quad \hat{b} = \frac{bP_0}{R_u T_0} = \sum_{i=1}^N X_i \hat{b}_i \longrightarrow \hat{b}_i = \frac{b_i P_0}{R_u T_0} = 0.08664 \frac{T_{ci}}{P_{ci}}
 \end{aligned}$$

- Now use Cardano's Method
- Solve for Normalized density

$$Z^3 - Z^2 + (A - B - B^2)Z - AB = 0$$

$$Z = \frac{P}{T\mathcal{R}} \quad \mathcal{R} = \frac{\rho R_u T}{P}$$

# ISENTROPIC FLOW

- Choose to vary Pressure

$$\frac{dT}{T} = \beta \frac{d\rho}{\rho} + \frac{1}{c_v + k} ds$$

$$\frac{dP}{P} = (f + g\beta) \frac{d\rho}{\rho} + \frac{1}{c_v + k} ds$$

$$f = \frac{2Z^3 - Z^2 + AB}{Z^3 - B^2Z}$$

$$g = \frac{1}{Z - B} - \frac{A'}{Z(Z + B)}$$

$$\beta = \frac{(\gamma - 1)Zg}{1 + \frac{k}{c_v}}$$

$$\frac{k}{c_v} = (\gamma - 1) \frac{A''}{B} \ln\left(\frac{Z + B}{Z}\right)$$

$$\frac{dU^2}{dP} = -\frac{2}{\mathcal{R}}$$

$$C = \sqrt{TZ(f + g\beta)}$$

$$\frac{d\alpha}{dP} = -\alpha \left[ \frac{1}{P(f + g\beta)} - \frac{1}{\mathcal{R}U^2} \right]$$

# ISENTROPIC FLOW

$$A' = \frac{dA}{dT} = T \frac{d\hat{a}}{dT} = \sum_{i=1}^N \sum_{j=1}^N \frac{1 - k_{ij}}{2} X_i X_j T \left[ \sqrt{\frac{\hat{a}_i}{\hat{a}_j}} \frac{d\hat{a}_j}{dT} + \sqrt{\frac{\hat{a}_j}{\hat{a}_i}} \frac{d\hat{a}_i}{dT} \right]$$

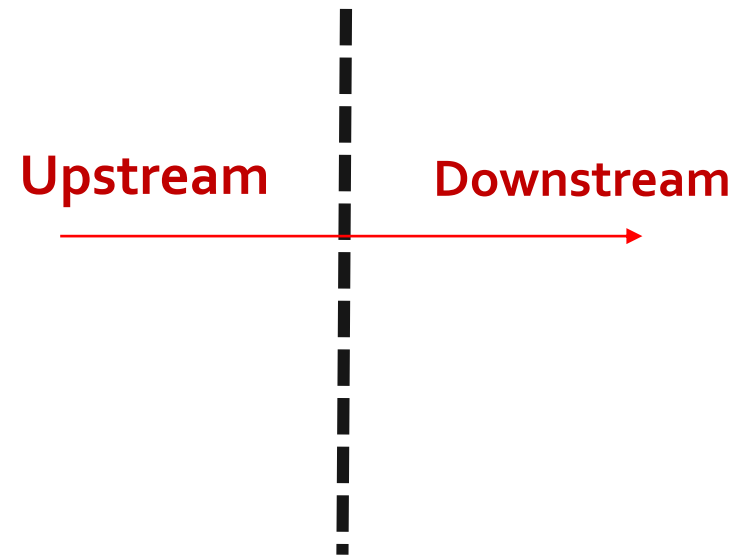
$$A'' = \frac{d^2 A}{dT^2} = T^2 \frac{d^2 \hat{a}}{dT^2} = \sum_{i=1}^N \sum_{j=1}^N \frac{1 - k_{ij}}{2} T^2 X_i X_j \left[ \sqrt{\frac{\hat{a}_i}{\hat{a}_j}} \frac{d^2 \hat{a}_j}{dT^2} + \frac{1}{\hat{a}_i \hat{a}_j} \frac{d\hat{a}_i}{dT} \frac{d\hat{a}_j}{dT} - \frac{1}{2} \frac{\hat{a}_i^{0.5}}{\hat{a}_j^{1.5}} \frac{d\hat{a}_j^2}{dT^2} + \sqrt{\frac{\hat{a}_j}{\hat{a}_i}} \frac{d^2 \hat{a}_i}{dT^2} - \frac{1}{2} \frac{\hat{a}_j^{0.5}}{\hat{a}_i^{1.5}} \frac{d^2 \hat{a}_i}{dT^2} \right]$$

$$\frac{d\hat{a}_i}{dT} = 0.42748 \frac{T_{ci}^{1.5}}{P_{ci} T^{0.5}} S_i \left[ 1 + S_i \left( 1 - \sqrt{\frac{T}{T_{ci}}} \right) \right]$$

$$\frac{d^2 \hat{a}_i}{dT^2} = - \frac{0.21374}{P_{ci}} \left( \frac{T_{ci}}{T} \right)^{1.5} S_i (1 + S_i)$$

# NORMAL SHOCK

- Five properties needed for full understanding of normal shock:
  - Pressure
  - Temperature
  - Velocity
  - Density
  - Enthalpy
- Two methods for normal shock calculation:
  - First upstream velocity not needed
  - Second upstream velocity needed



# NORMAL SHOCK – METHOD ONE

- Ten total properties
- 4 Known
  - $T_1, P_1, Z_1, h_1$
- 6 Unknown
  - $T_2, P_2, Z_2, h_2, U_1, U_2$
- 5 Equations

$$\rho_1 u_1 = \rho_2 u_2$$

$$\rho_1 u_1^2 + P_1 = \rho_2 u_2^2 + P_2$$

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2}$$

$$h = h_{ideal} + \frac{1}{MW} \left[ R_u T (Z - 1) + \frac{T \frac{da}{dT} - a}{b} \ln \frac{Z + B}{Z} \right]$$

$$h_{ideal} = C_p T$$

$$Z^3 - Z^2 + (A - B - B^2)Z - AB = 0$$

# NORMAL SHOCK – METHOD ONE

- Choose Temperature Ratio:  $T_2$
- Guess a Pressure Ratio:  $P_2$ 
  - Use Cardano's Method to solve for compressibility:  $Z_2$
  - Solve for density:  $\rho_2$
  - Manipulate momentum and continuity to solve for velocity:  $u_1$
  - Use continuity to get velocity:  $u_2$
  - Using literature defined equation solve for enthalpy:  $h_1$
  - Check solution using Total Enthalpy
- If total enthalpy's math  $T_2$ ,  $P_2$  combination matches

$$\rho_1 u_1 = \rho_2 u_2$$

$$\rho_1 u_1^2 + P_1 = \rho_2 u_2^2 + P_2$$

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2}$$

$$Z^3 - Z^2 + (A - B - B^2)Z - AB = 0$$

$$h = h_{ideal} + \frac{1}{MW} \left[ R_u T (Z - 1) + \frac{T \frac{da}{dT} - a}{b} \ln \frac{Z + B}{Z} \right]$$
$$h_{ideal} = C_p T$$

# NORMAL SHOCK – METHOD TWO

**This time upstream velocity is known**

**Guess  $T_r$ :**

Ignore upstream velocity for now

Go through Method One

Now have all upstream and downstream conditions

Compare  $U_1$  found via Method One to  $U_1$  defined  
by upstream conditions

# RESULTS COMPUTATIONAL COST

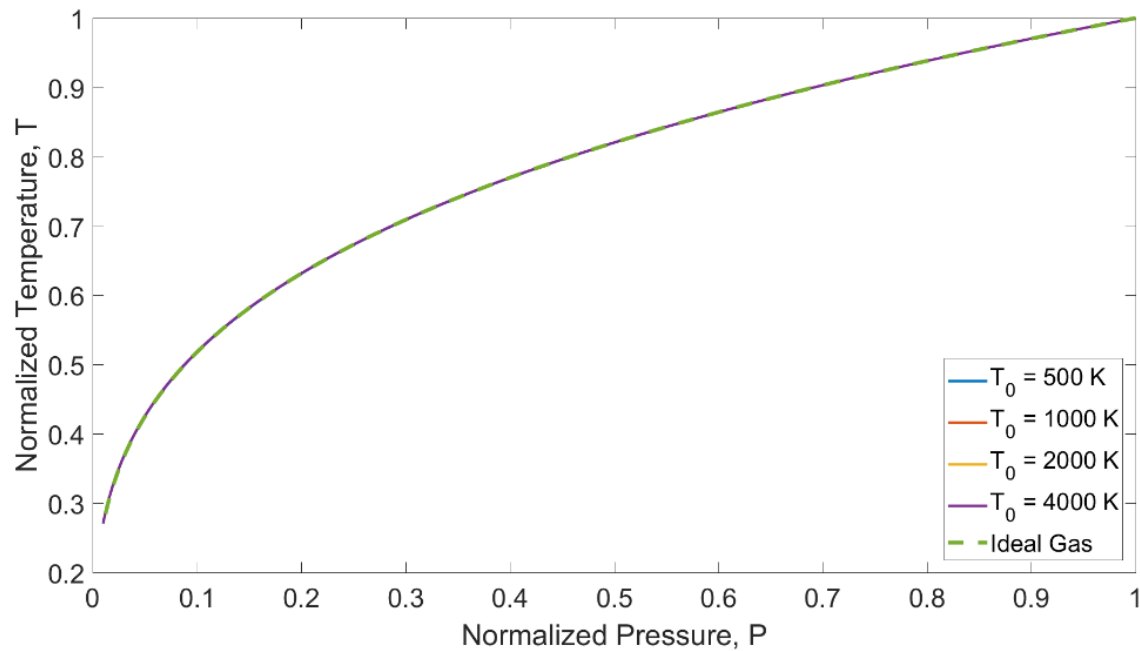
- Use Normalized Values
- Had computer run through all of calculations 52 times

	Root Function	Approximate Solution
Computational Cost	2.0454	0.0327

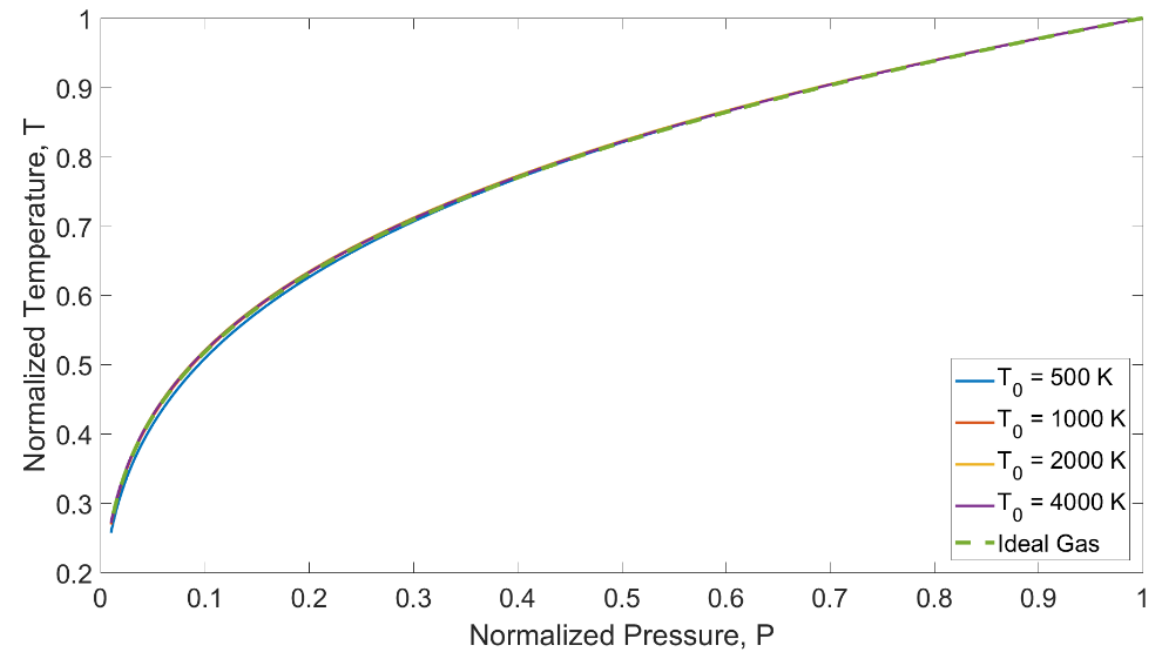


# RESULTS ISENTROPIC FLOW

10 bar

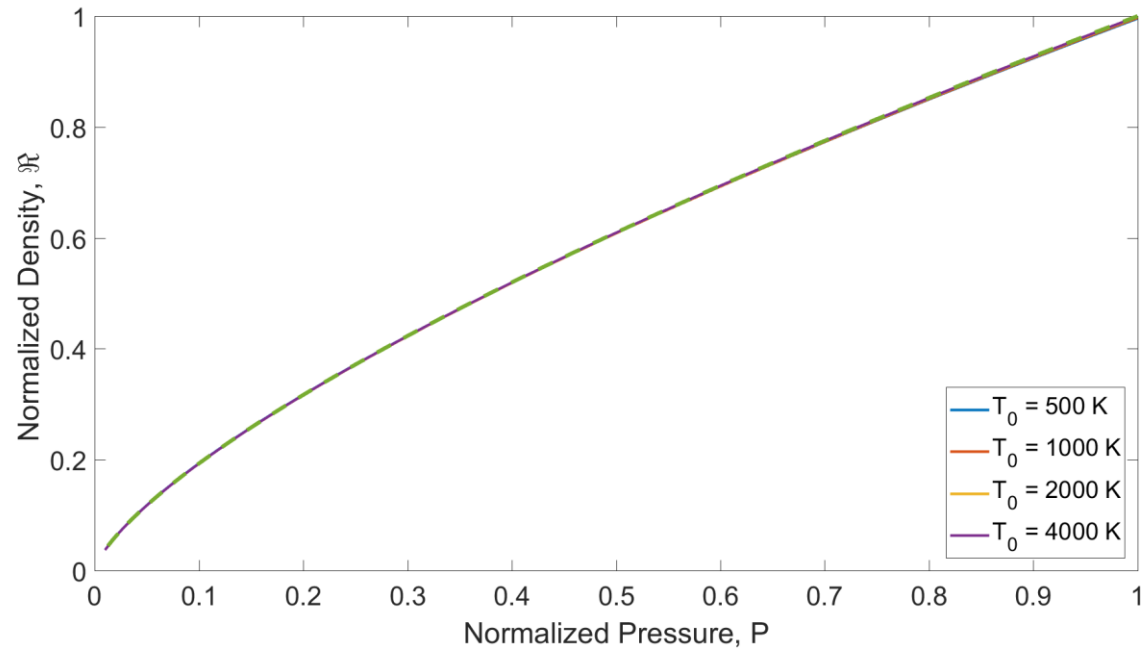


500 bar

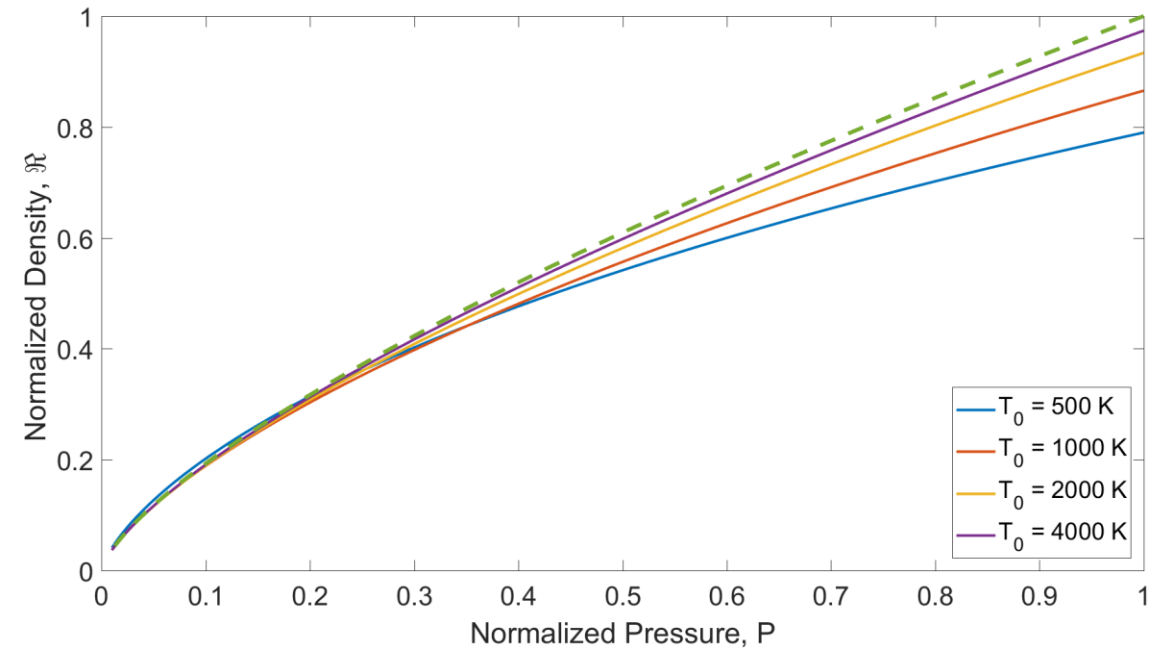


# RESULTS ISENTROPIC FLOW

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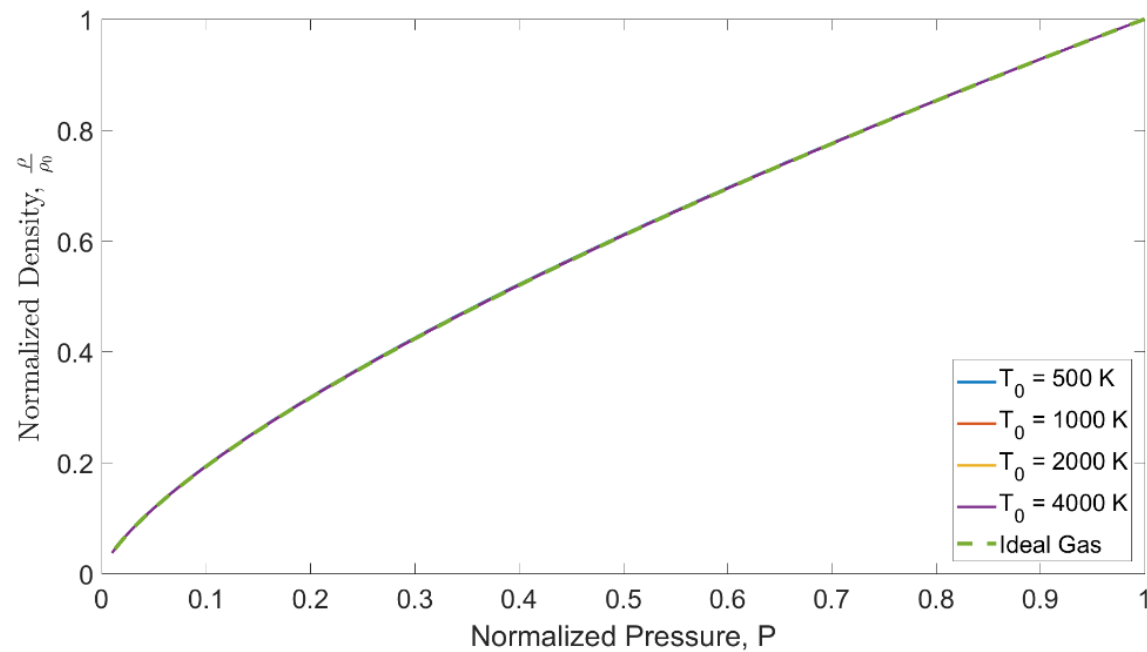


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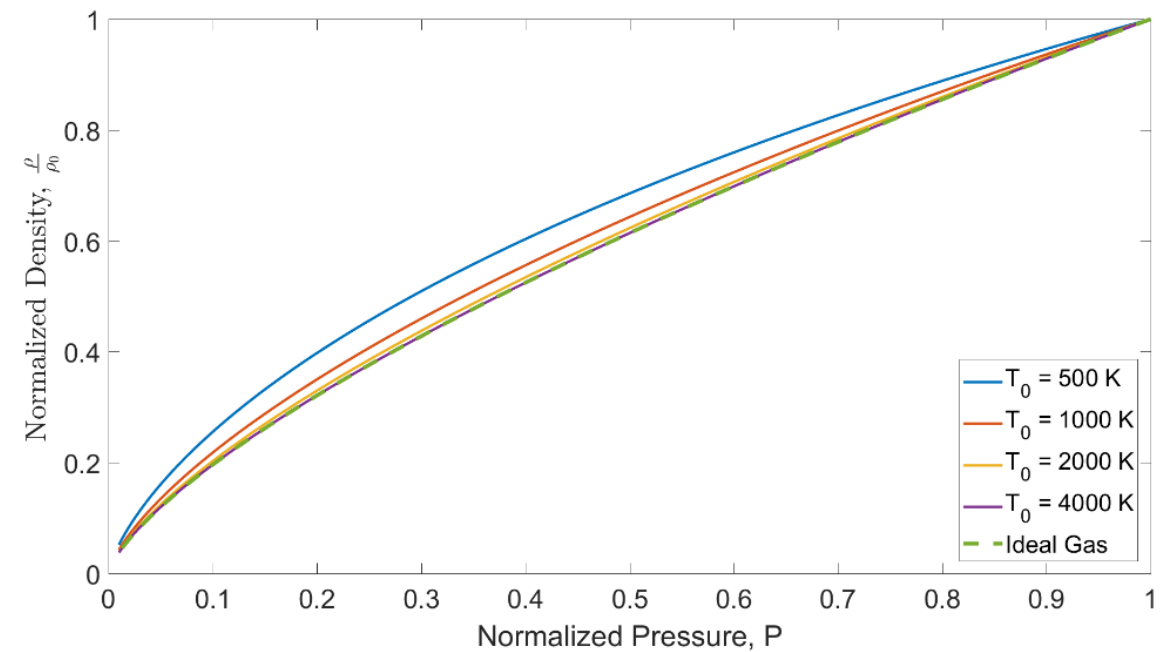


# RESULTS ISENTROPIC FLOW

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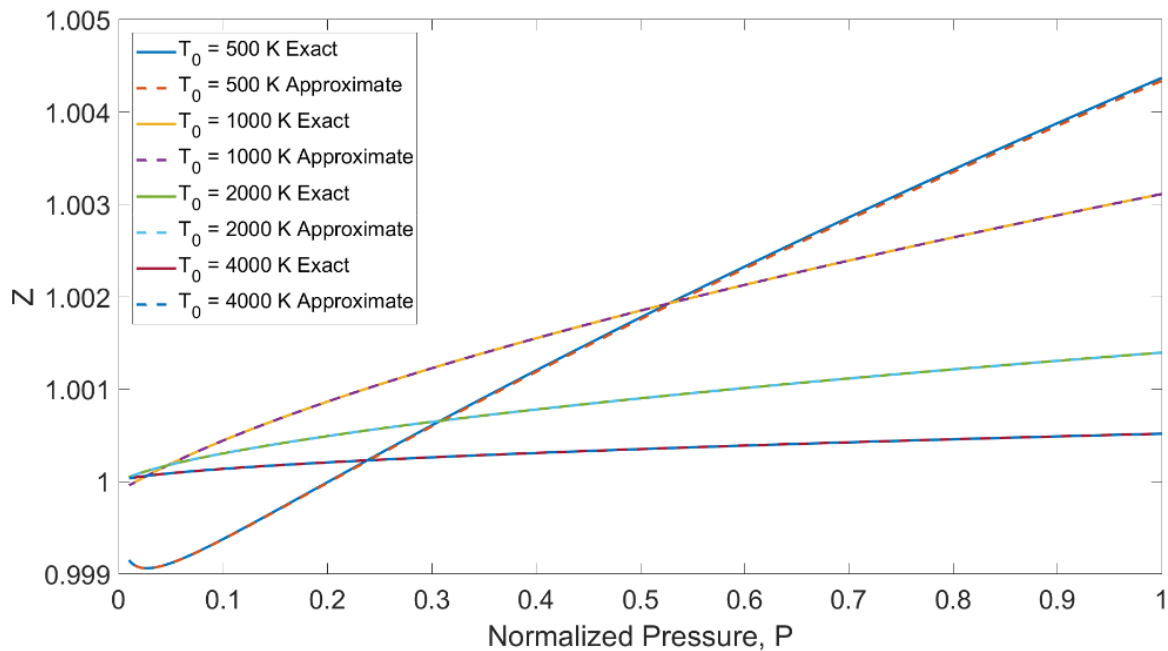


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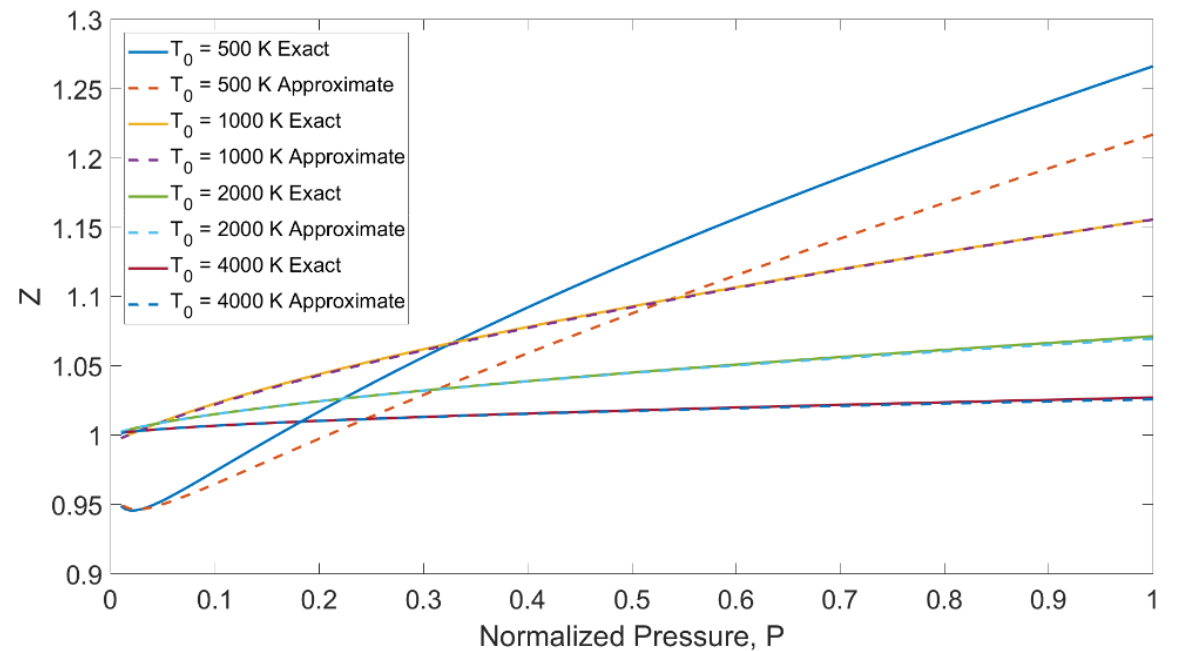


# RESULTS ISENTROPIC FLOW

**10 bar**

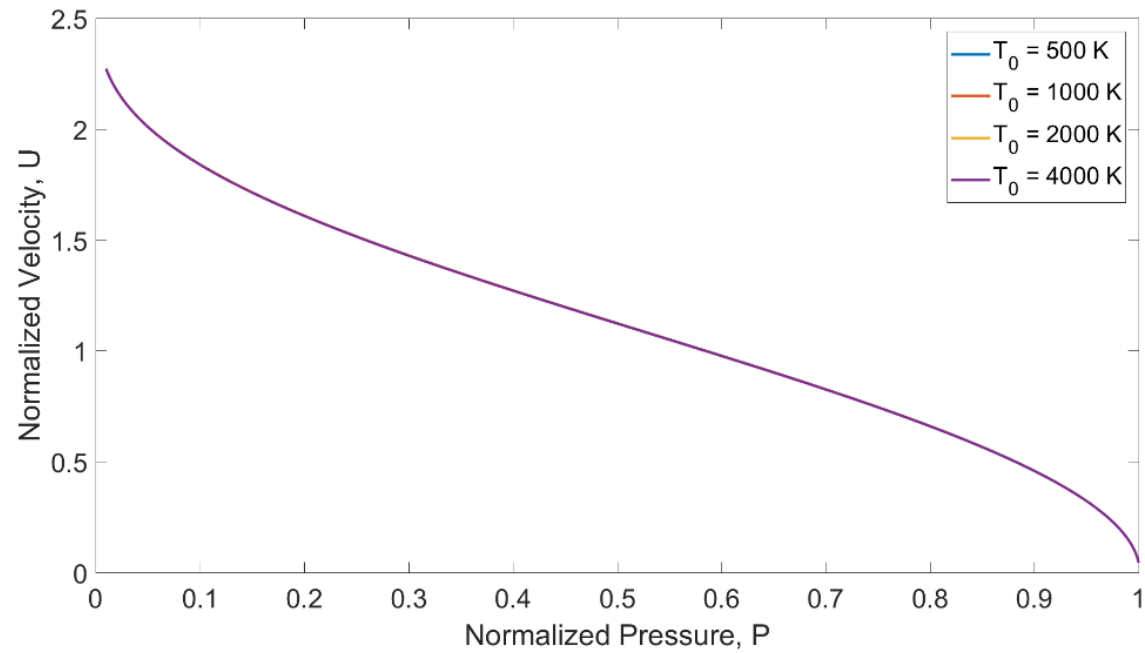


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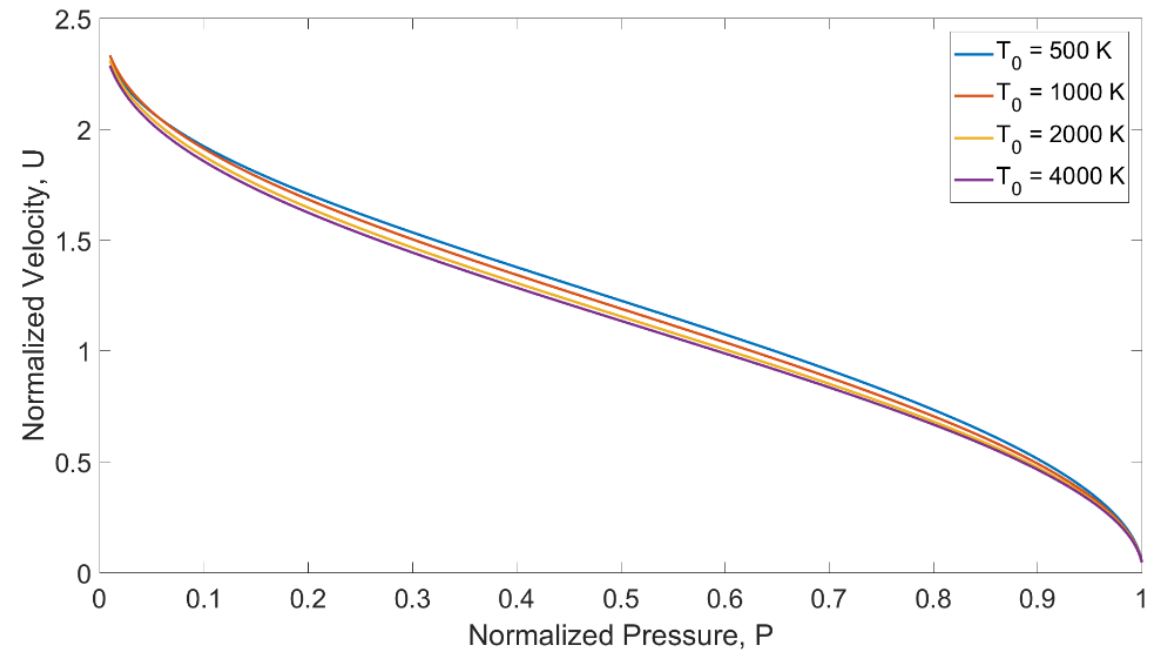


# RESULTS ISENTROPIC FLOW

10 bar

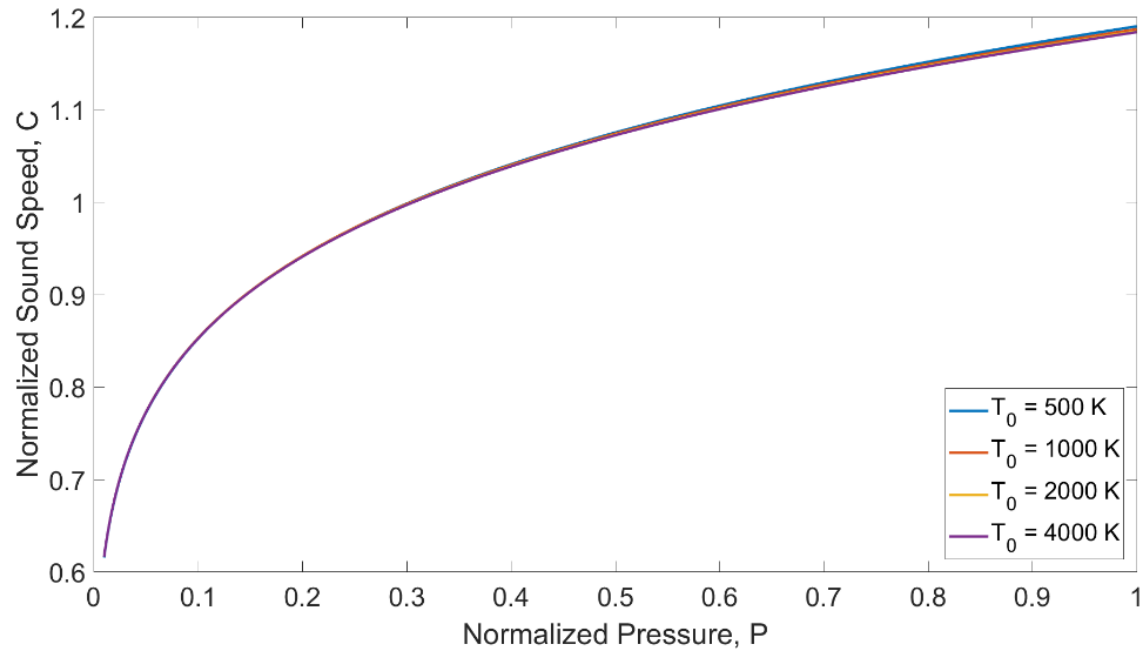


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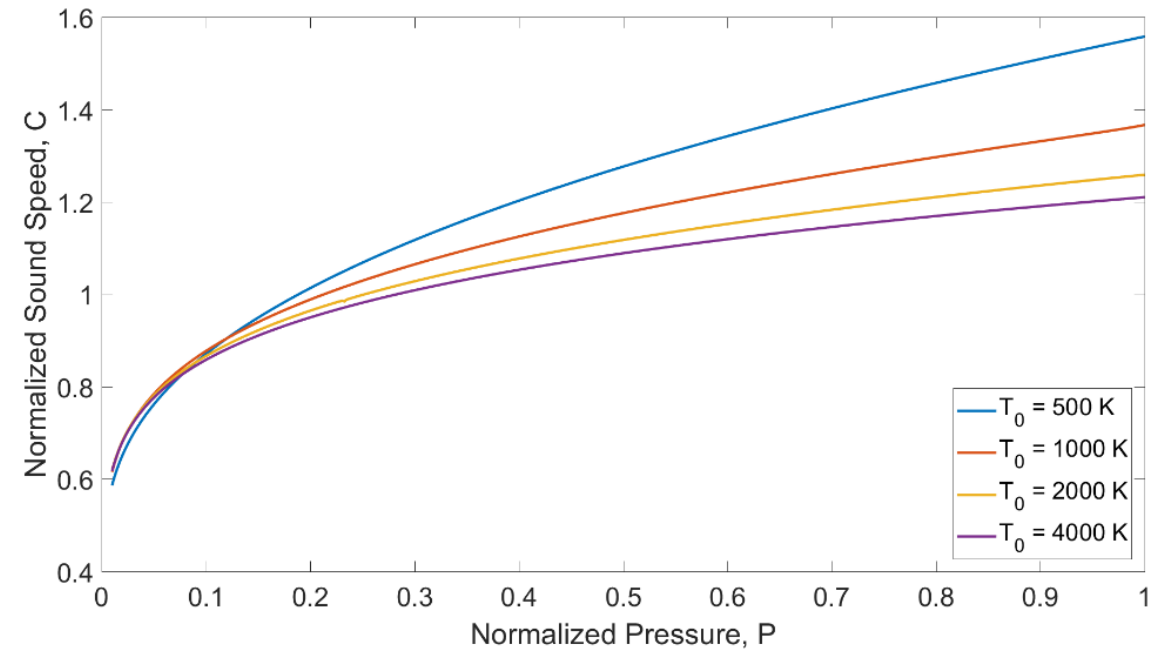


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10 bar

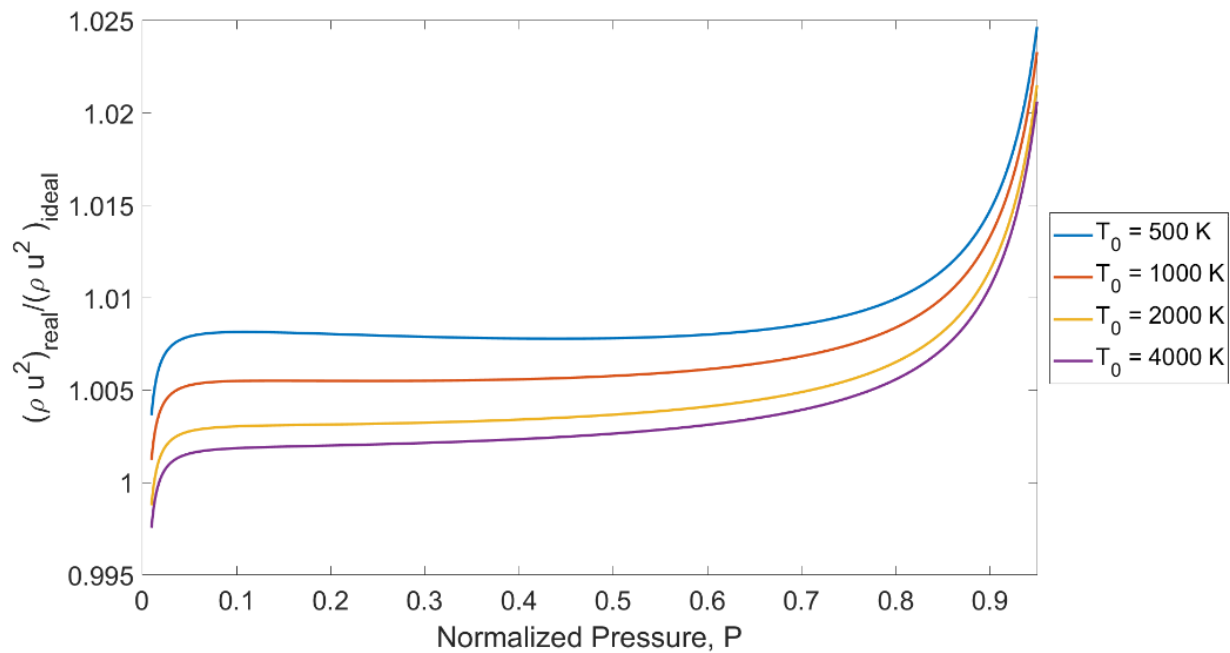


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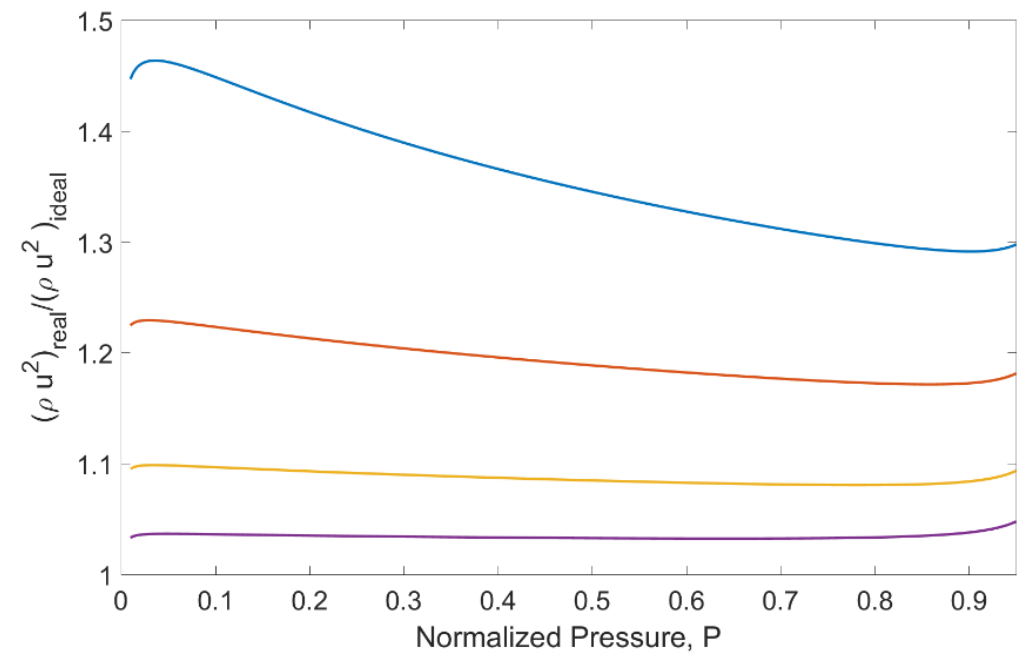


# RESULTS ISENTROPIC FLOW

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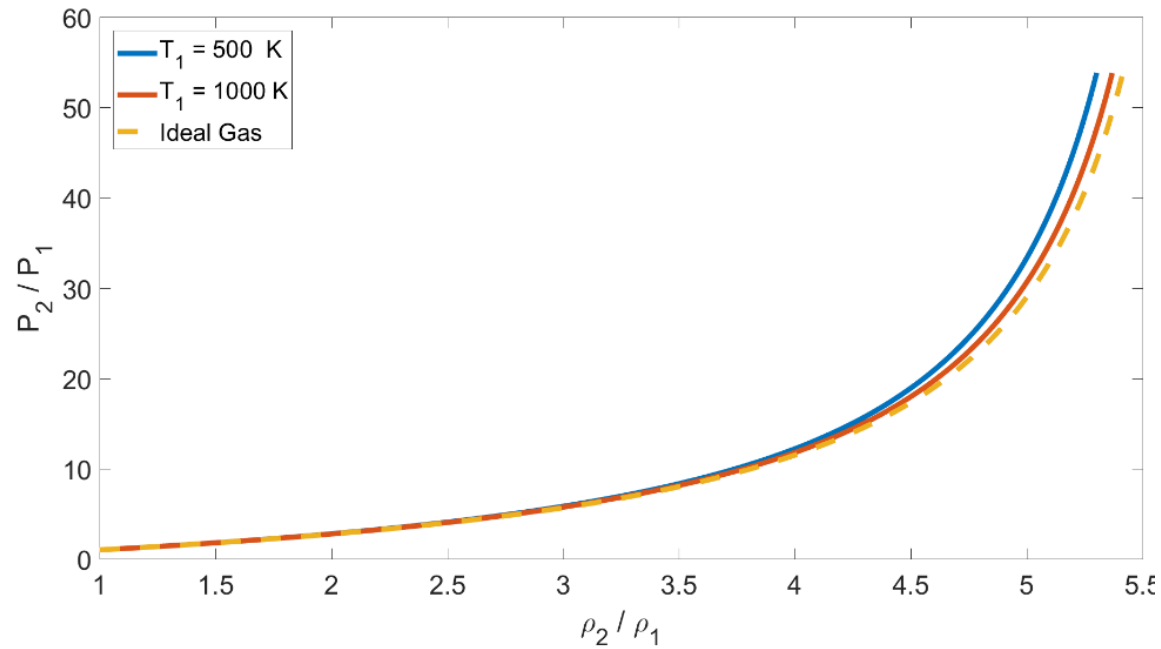


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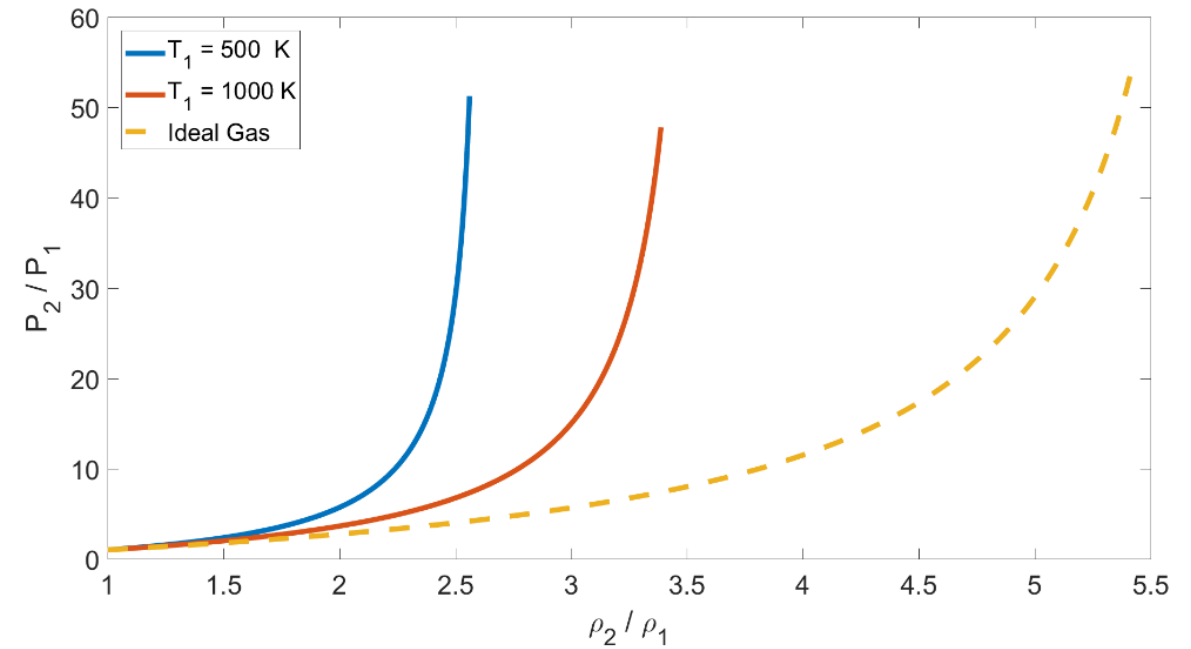


# RESULTS NORMAL SHOCK

10 bar

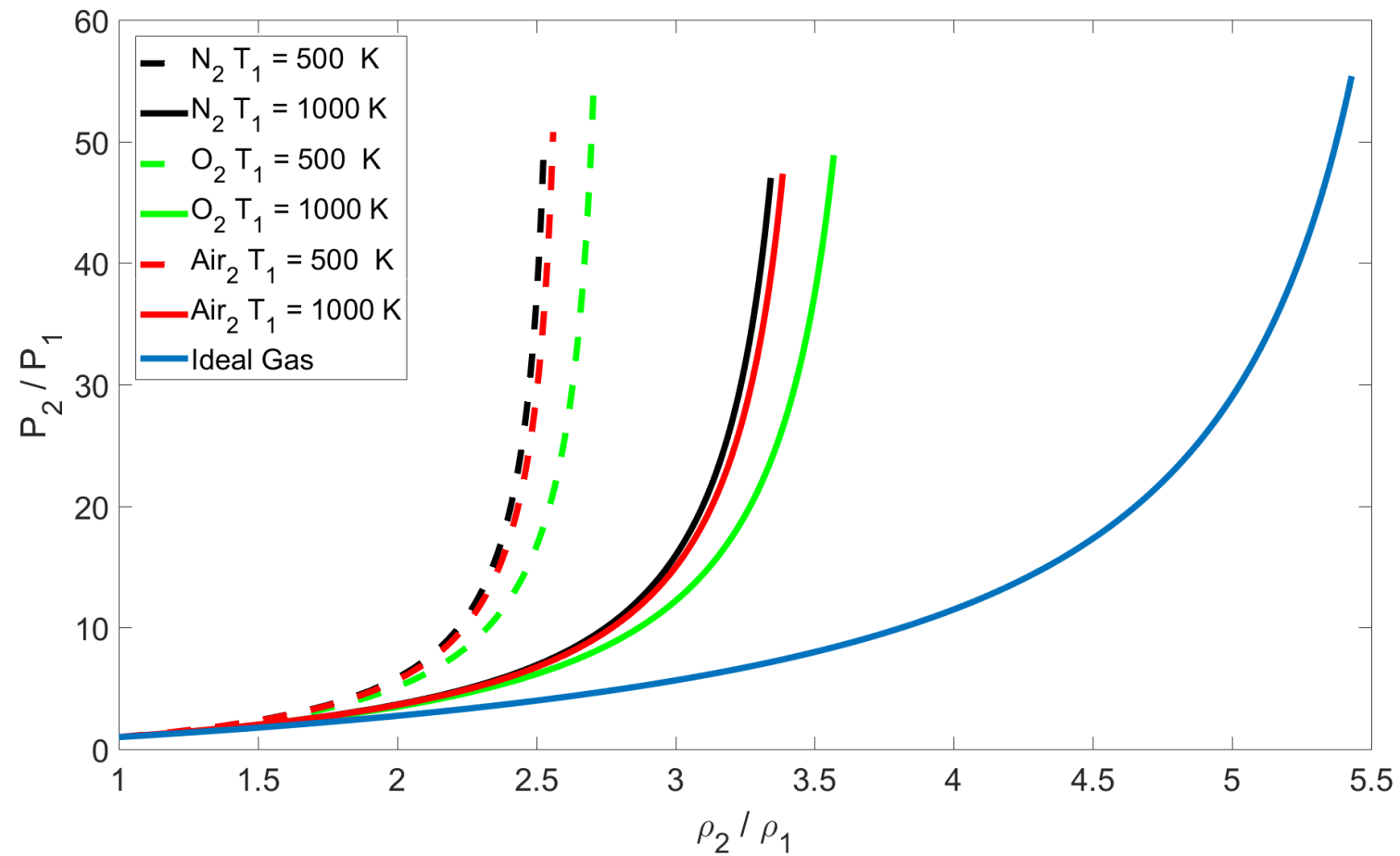


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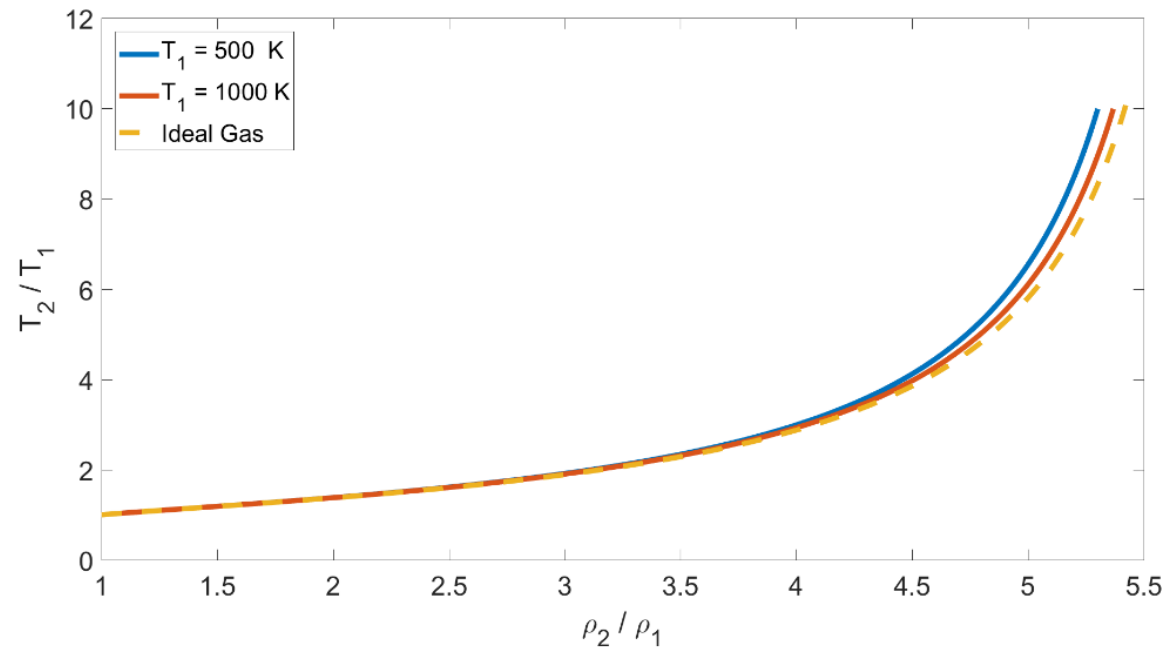


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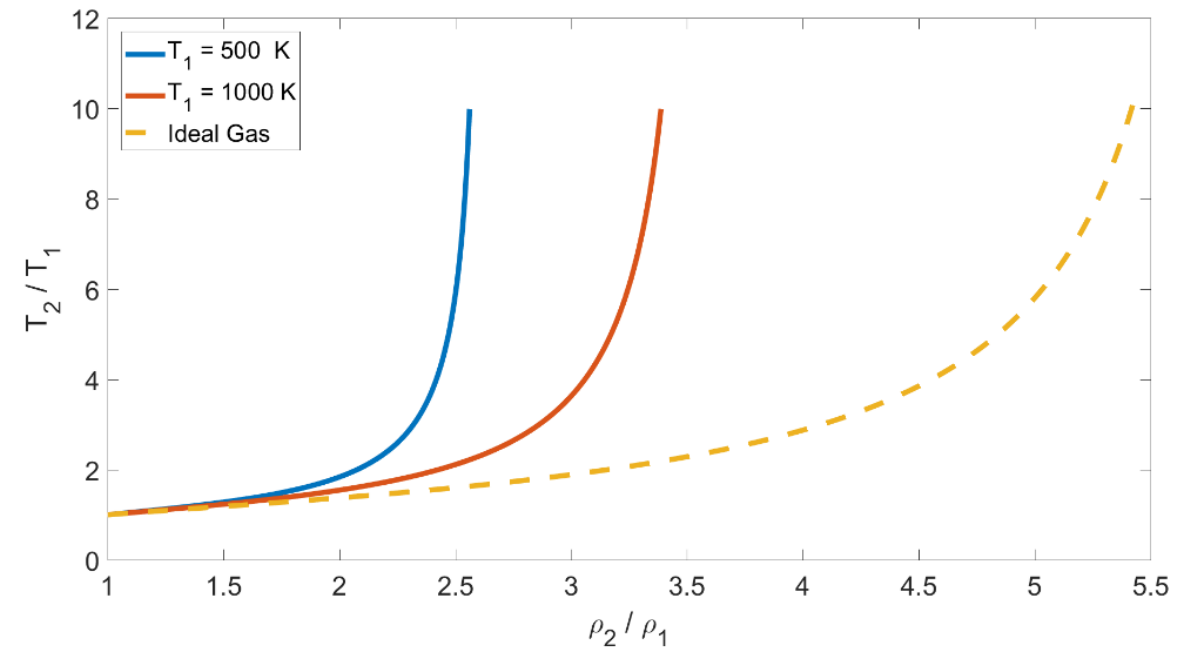


# RESULTS NORMAL SHOCK

10 bar

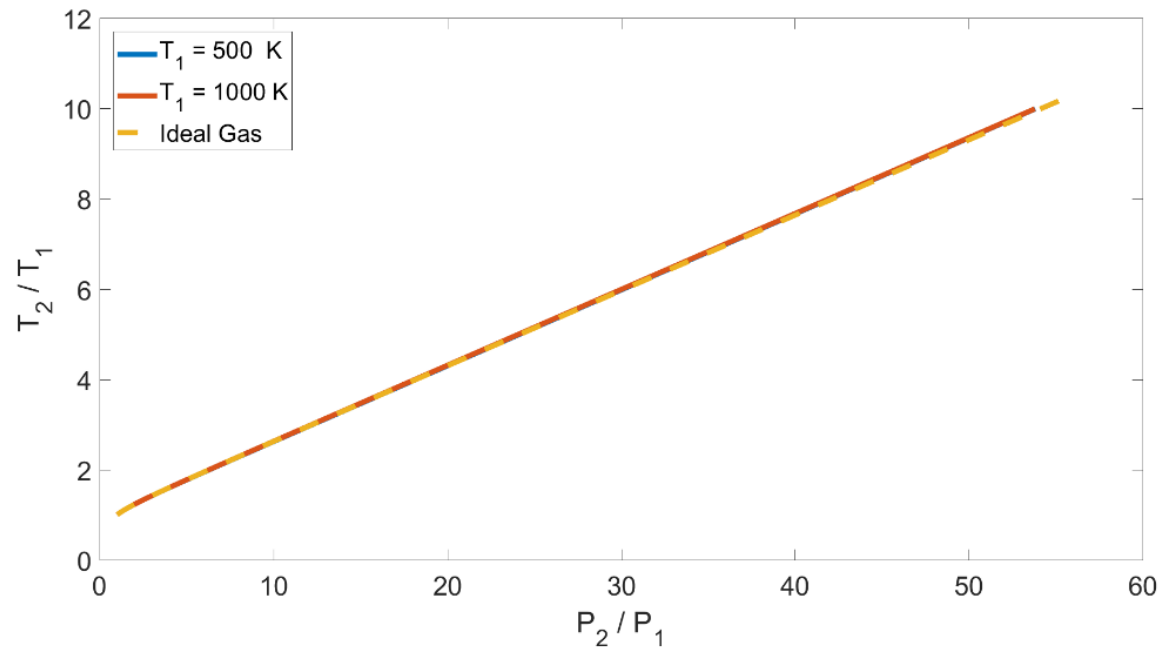


500 bar

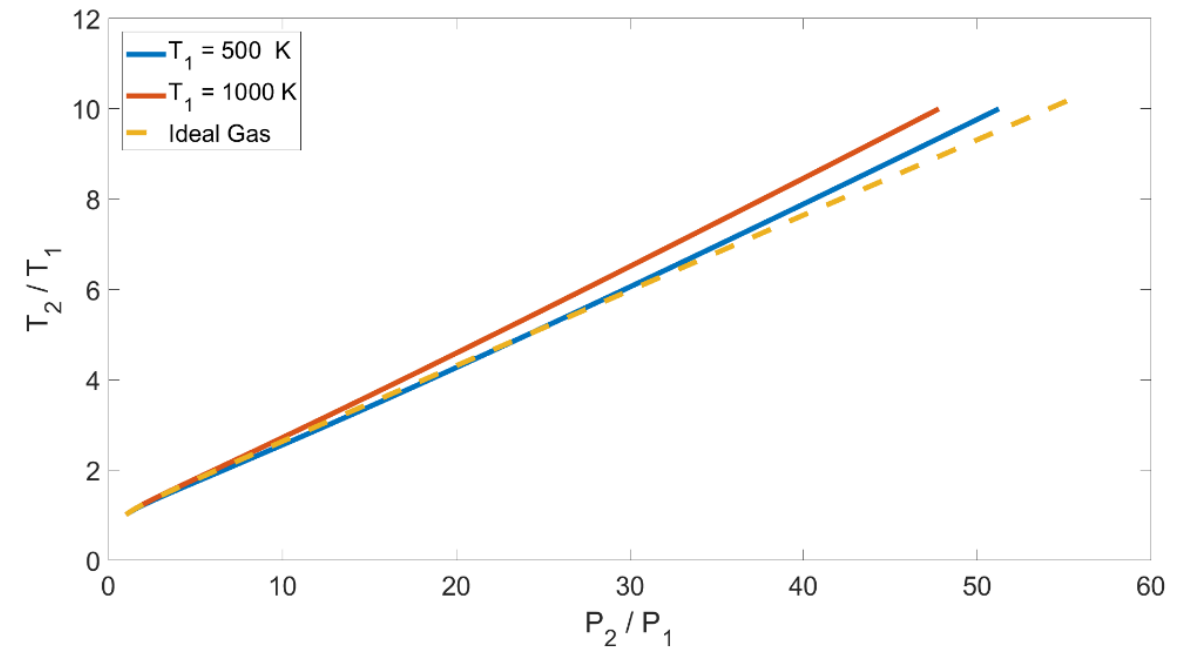


# RESULTS NORMAL SHOCK

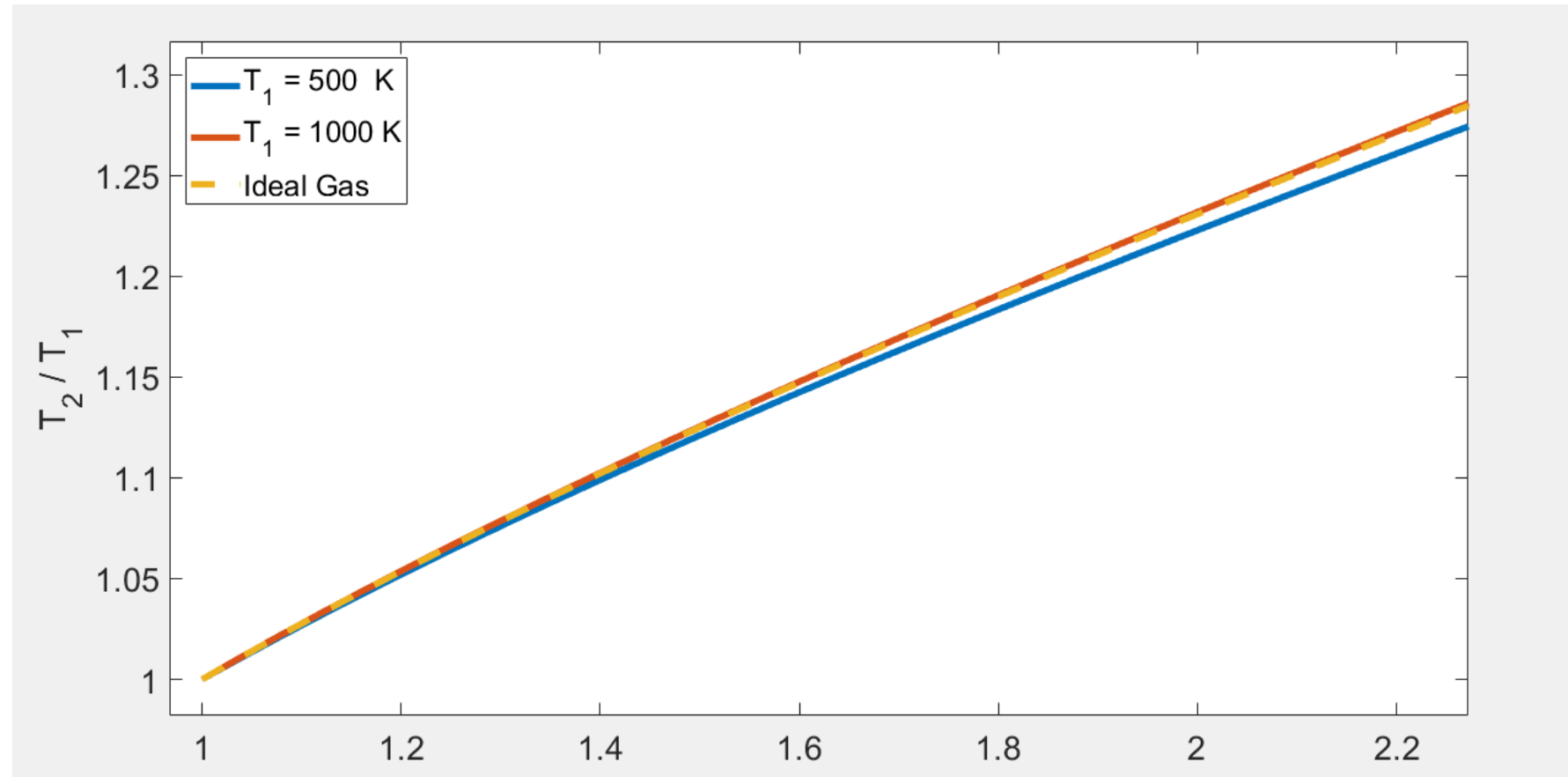
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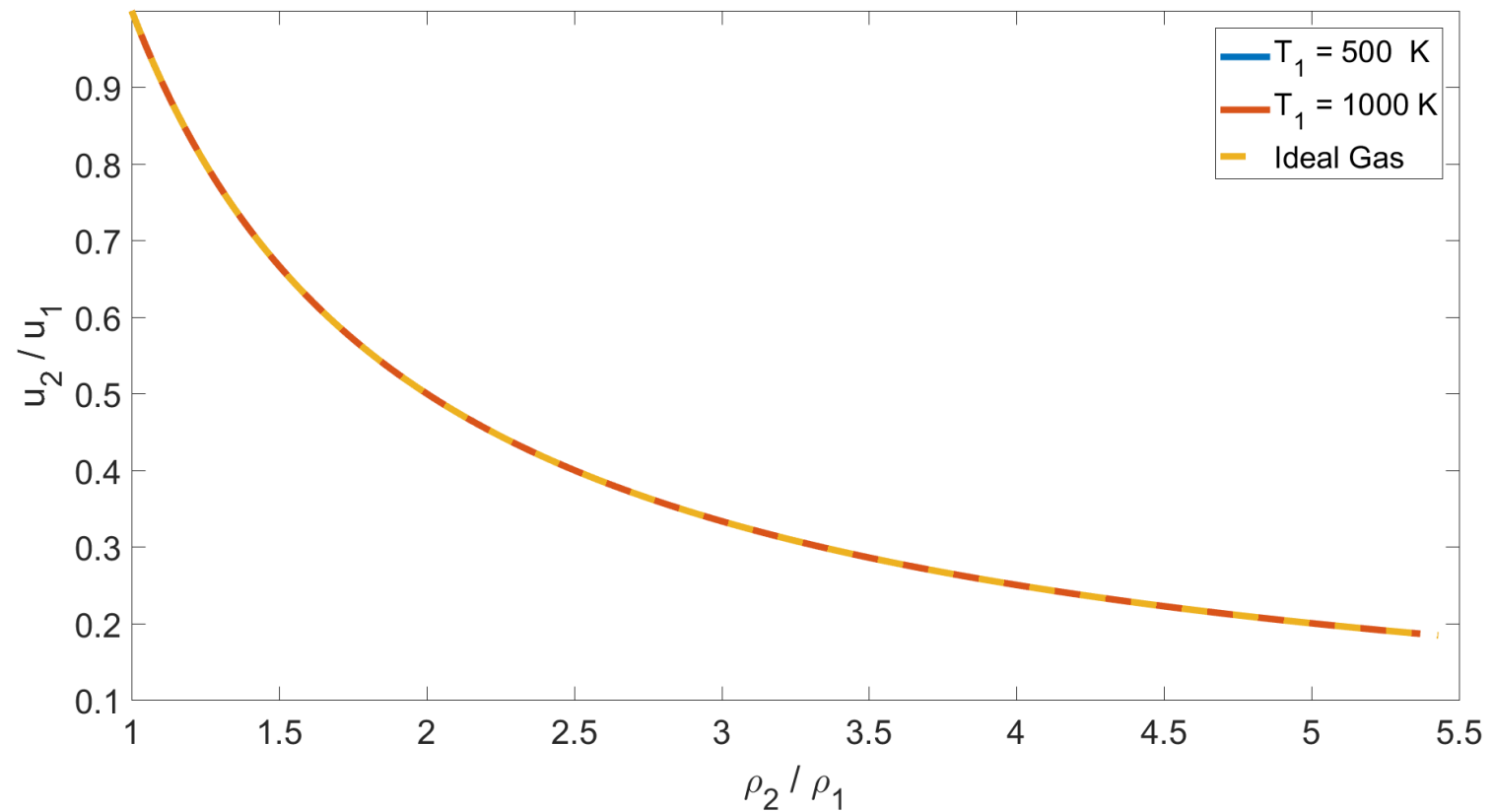
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# RESULTS NORMAL SHOCK



# RESULTS NORMAL SHOCK



# RESULT SUMMARY – MAX DEVIATION

Temperature – 4.25%

Density – 28.19%

Mass Flux – 3.25%

## Recap:

Used Soave-Redlich-Kwong EoS

Defined method for solving cubic equation directly

Defined method for calculating isentropic flow

Defined method for finding normal shock

Showed Results

## Future Studies:

Focus on higher pressures and temperatures

Explore more values for binary interaction coefficient

Introduce more temperature dependent terms

# CLOSING REMARKS

THANK YOU





QUESTIONS