

# Combustion Analysis Report

## Input Parameters:

Fuel: Methanol (CH3OH) [simplified]

Initial temperature (T): 800.0 K

Pressure (P): 2.0 atm

Equivalence ratio (phi): 1.0

Grid Size (NxN): 4x4

Oxidizer: Air

## Calculation Statistics:

Total points calculated: 16

Total calculation time: 440.92 seconds

## Outlier Compensation Settings:

Parameters used for outlier compensation:

Parameter	Threshold	Multiplier
T_ad	3500.0	3.0
ignition_delay	100000.0	3.0
flame_speed	100.0	3.0
NOx	20000.0	3.0
CO	75000.0	3.0
CO2	200000.0	3.0

Advanced Simulation Settings:

Configured parameters for simulation mechanisms:

Parameter	Value	Unit
ignition_end_time	0.1	s
ignition_temp_threshold	100	K
ignition_detection_method	max_dTdt	
ignition_detection_species	OH	
flame_width	0.05	m

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Results directory: C:\Users\warsa\Desktop\6SEM\MKWS\COMBI\_BUMBI\_v5 FINAL\Calc\_Results\_1

# Important Notes on Physical Realism

## Ignition Delay Plots:

- Extremely short or zero delay times may indicate non-ignition within simulation time
- At low temperatures or pressures, ignition may not occur, leading to reported 0.0 values
- True zero ignition delay is non-physical as there's always finite time for reactions
- Flat areas at zero likely indicate conditions outside flammability limits
- Current detection method: max\_dTdt (Species: OH)

## NOx Emission Plots:

- Equilibrium calculations often overpredict real-world NOx emissions
- NOx formation is kinetically limited and may not reach equilibrium in practical systems
- Factors like flame quenching limit actual NOx below equilibrium predictions

## CO and CO2 Emission Plots:

- Equilibrium calculations might not reflect real emissions due to kinetic limitations
- CO may be underpredicted in rich conditions due to incomplete combustion
- CO2 may be overpredicted in systems with rapid quenching preventing full oxidation
- At extreme equivalence ratios, emissions are highly sensitive to kinetic factors

## Flame Speed Plots:

- Zero flame speeds indicate non-convergence, likely outside flammability limits
- At low temperatures or pressures, flames may be unstable or extinguish
- Abrupt changes in plots may indicate numerical boundaries of model validity
- Current flame width setting: 0.05 m

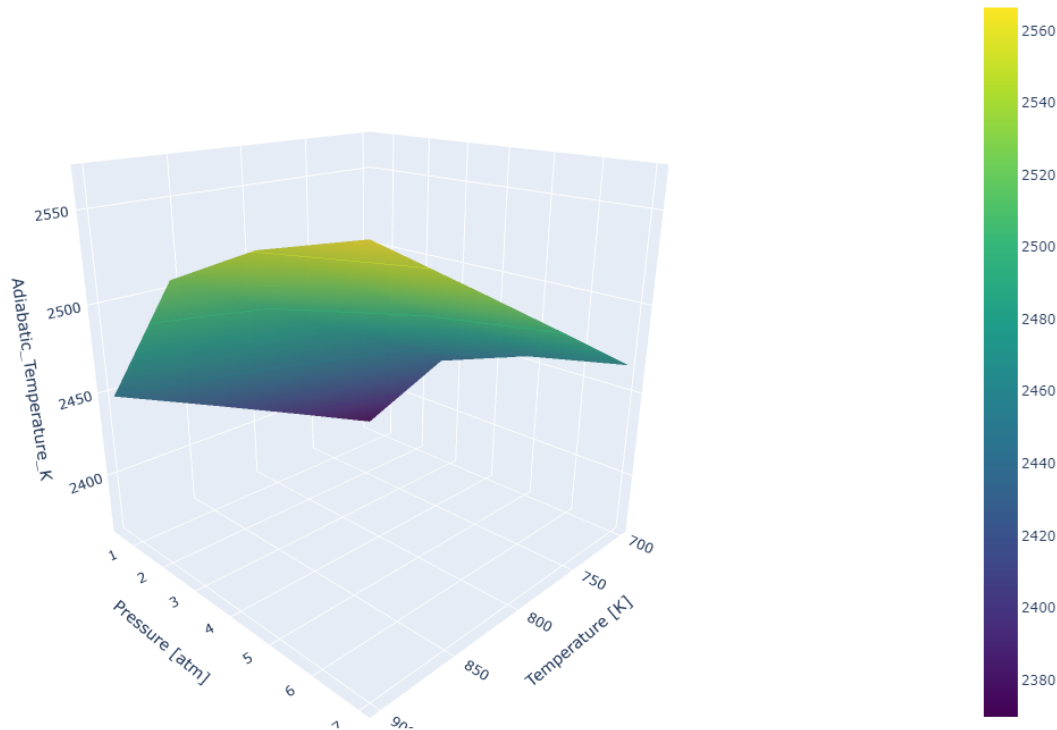
## General Interpretation Guidelines:

- Flat areas at zero often indicate non-ignition or non-propagation conditions
- Uniformly low/high values may represent model limitations in extreme regimes
- Abrupt changes may indicate boundaries where solver converges/fails
- Results at extreme conditions ( $T < 900\text{K}$ ,  $P < 1\text{atm}$ ,  $\phi < 0.5$  or  $\phi > 2.0$ ) may be unreliable

# 3D Plot: Adiabatic\_Temperature\_K

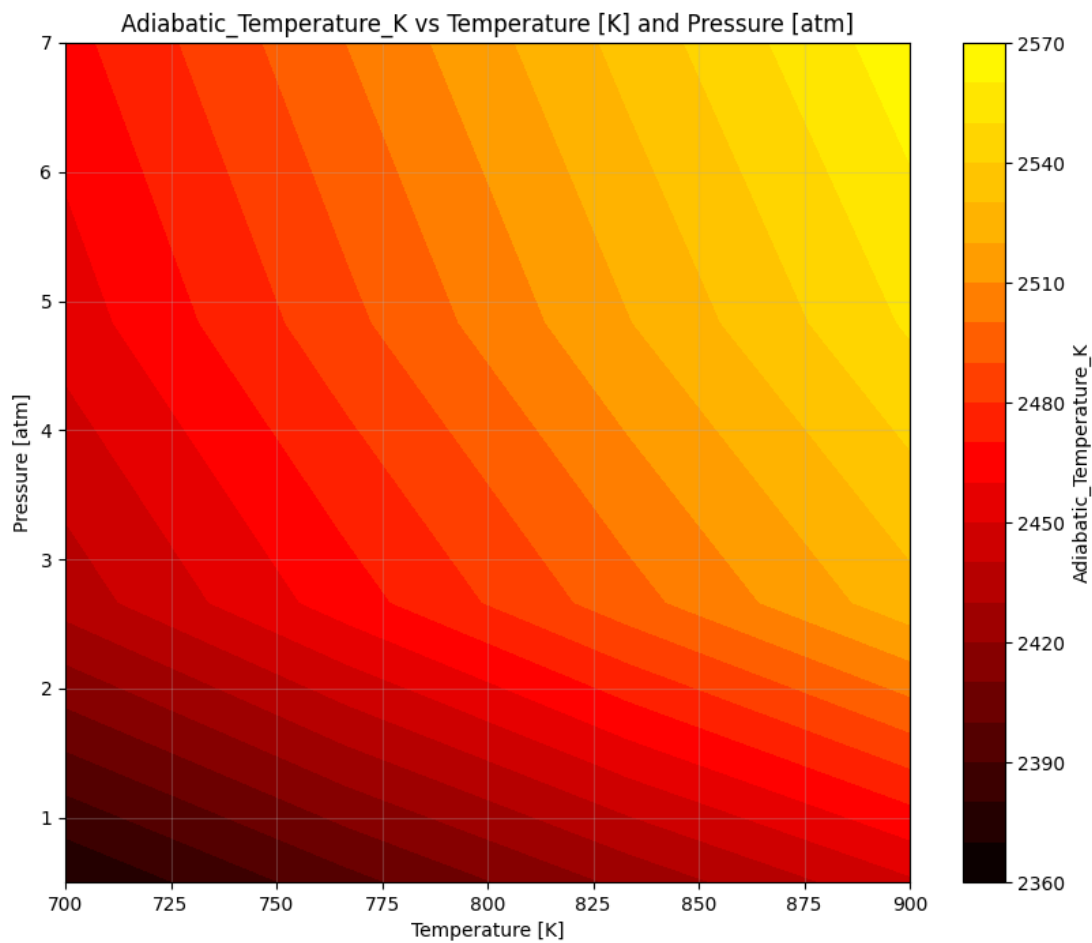
Temperature achieved during adiabatic combustion

Adiabatic\_Temperature\_K vs Temperature [K] and Pressure [atm]



# Contour Plot: Adiabatic\_Temperature\_K

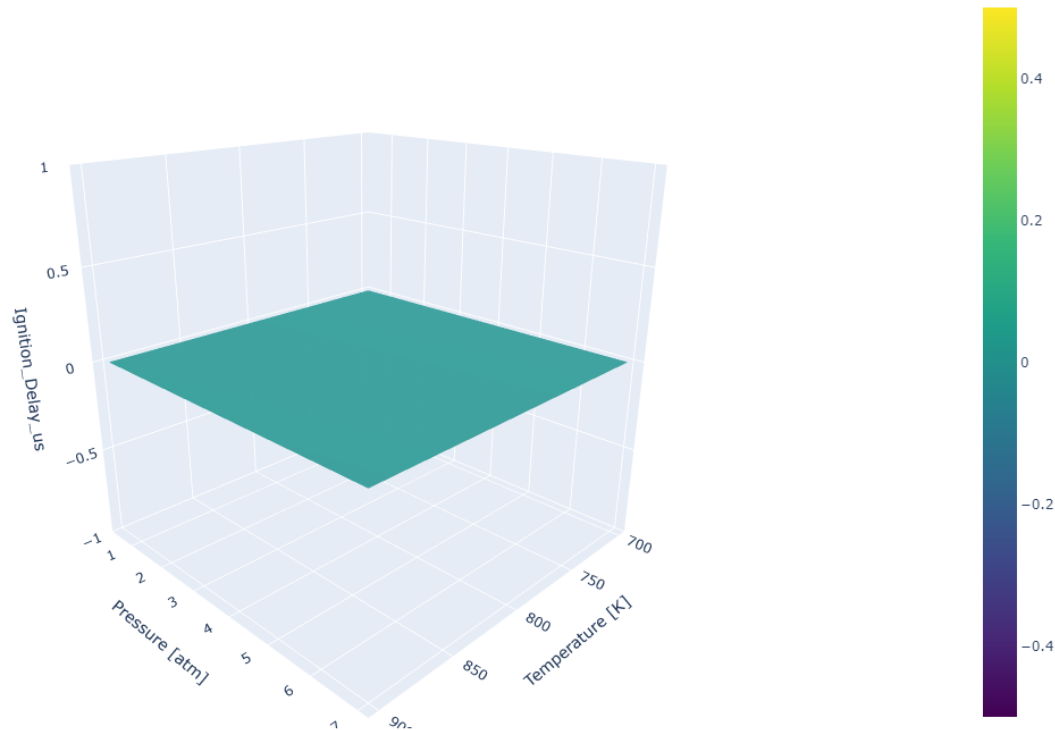
Temperature achieved during adiabatic combustion



# 3D Plot: Ignition\_Delay\_us

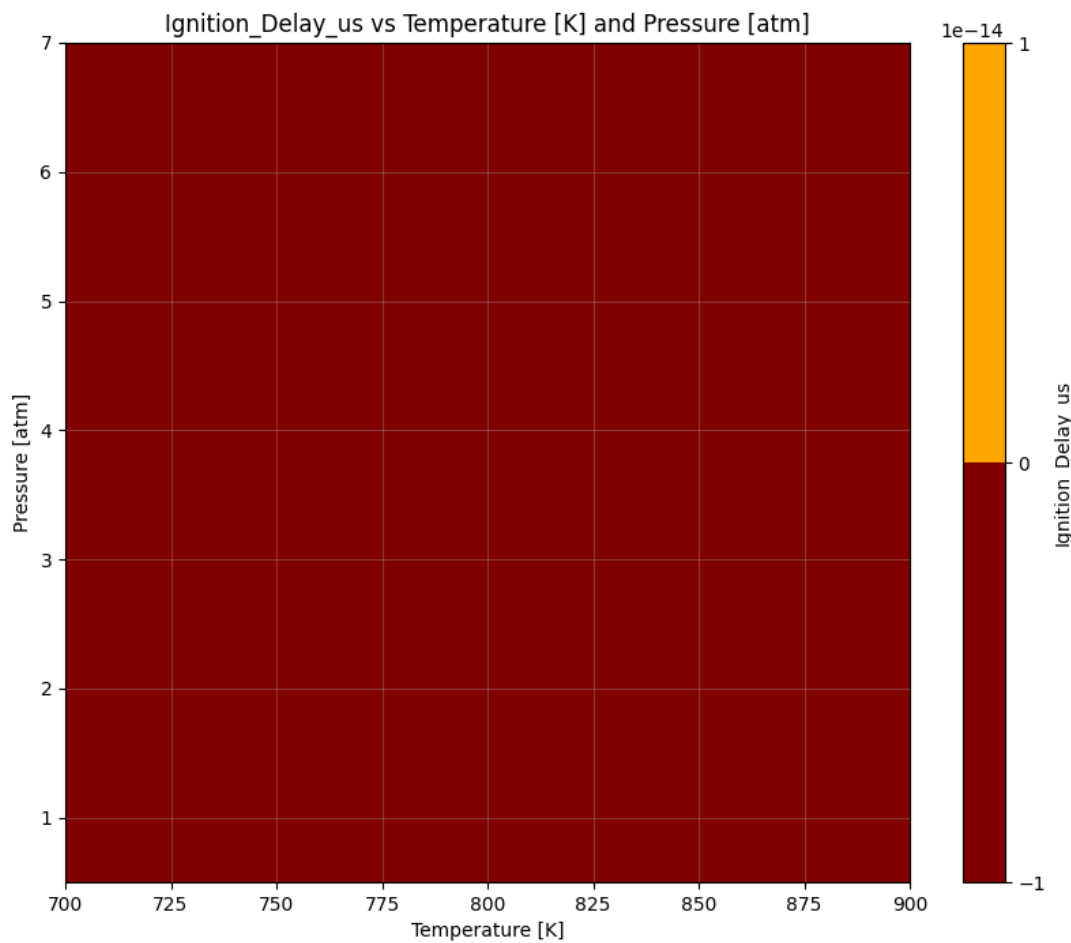
Time required for autoignition after heating

Ignition\_Delay\_us vs Temperature [K] and Pressure [atm]



# Contour Plot: Ignition\_Delay\_us

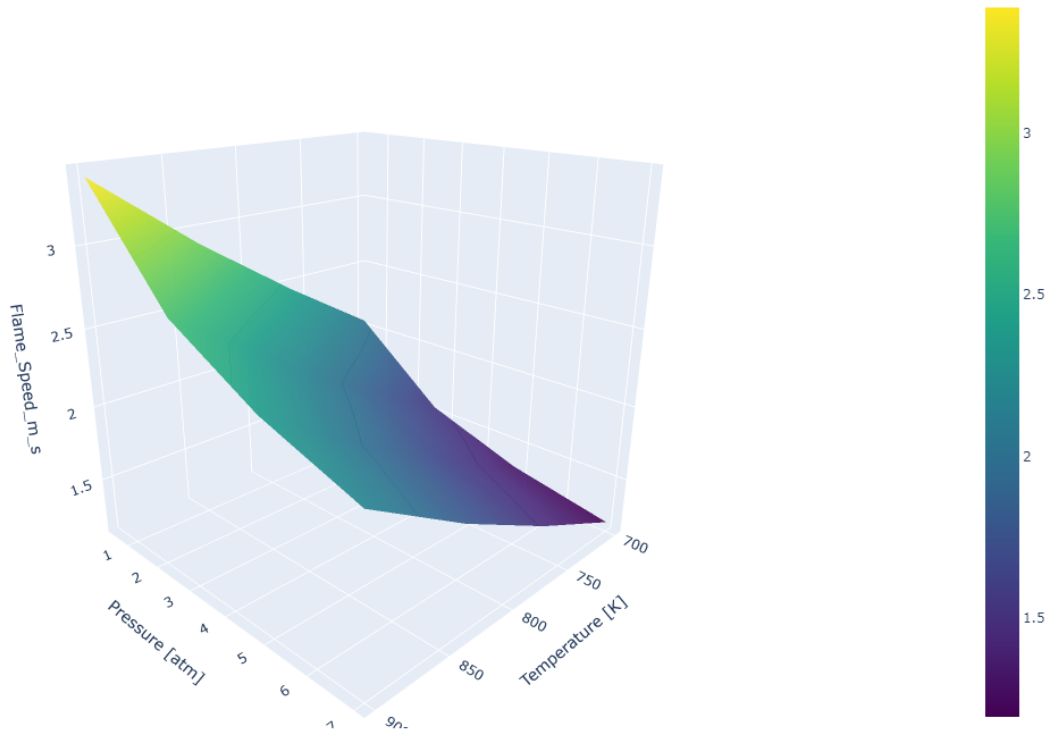
Time required for autoignition after heating



# 3D Plot: Flame\_Speed\_m\_s

Flame propagation speed in laminar conditions

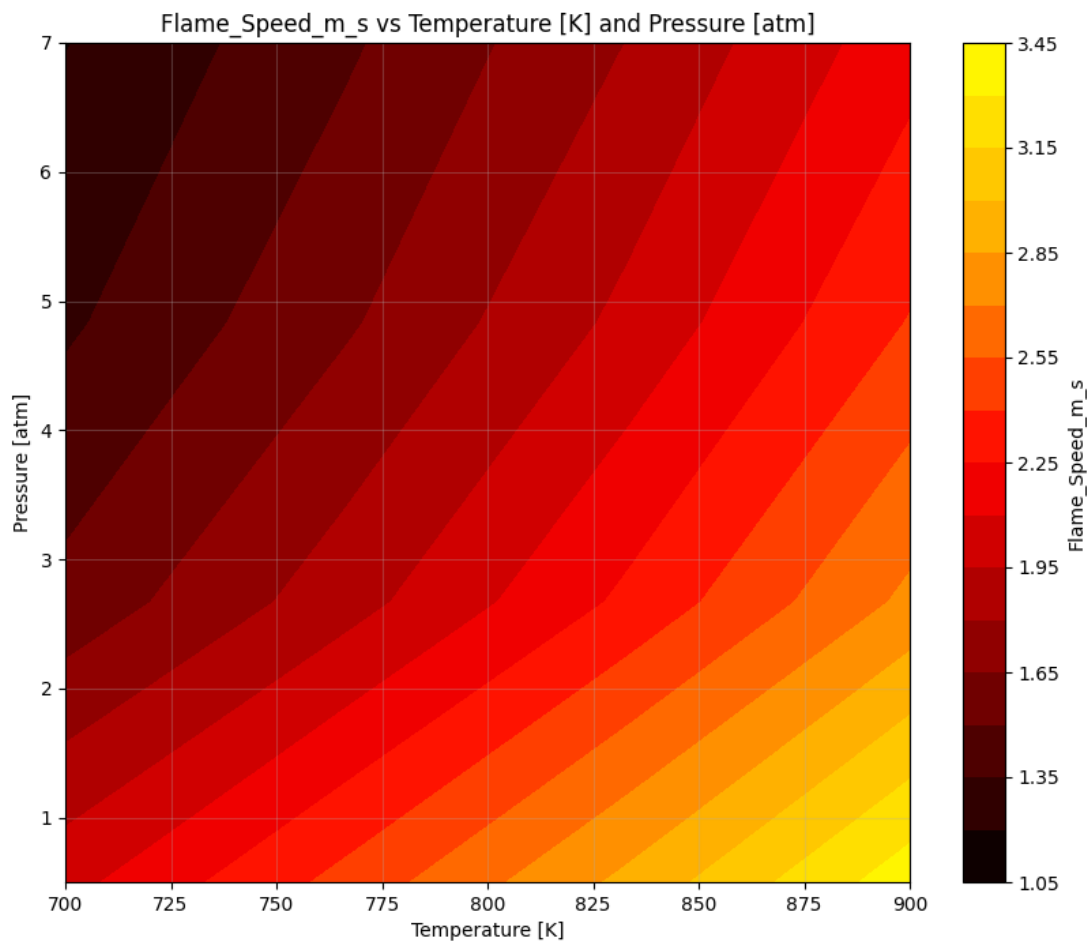
Flame\_Speed\_m\_s vs Temperature [K] and Pressure [atm]





# Contour Plot: Flame\_Speed\_m\_s

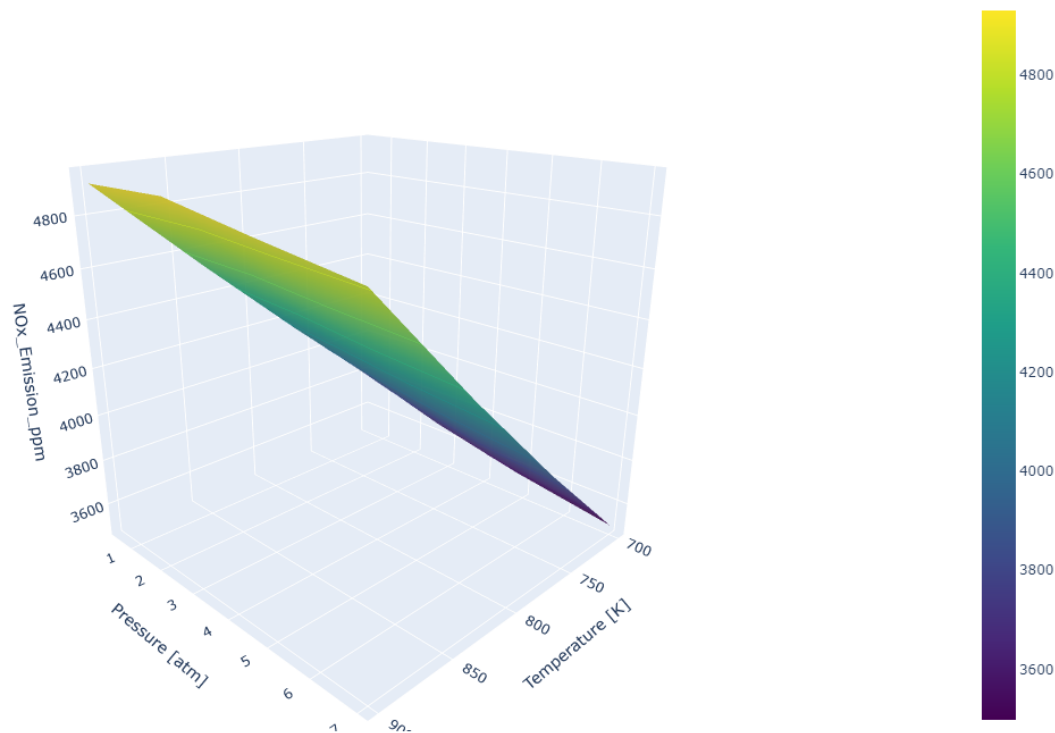
Flame propagation speed in laminar conditions



# 3D Plot: NOx\_Emission\_ppm

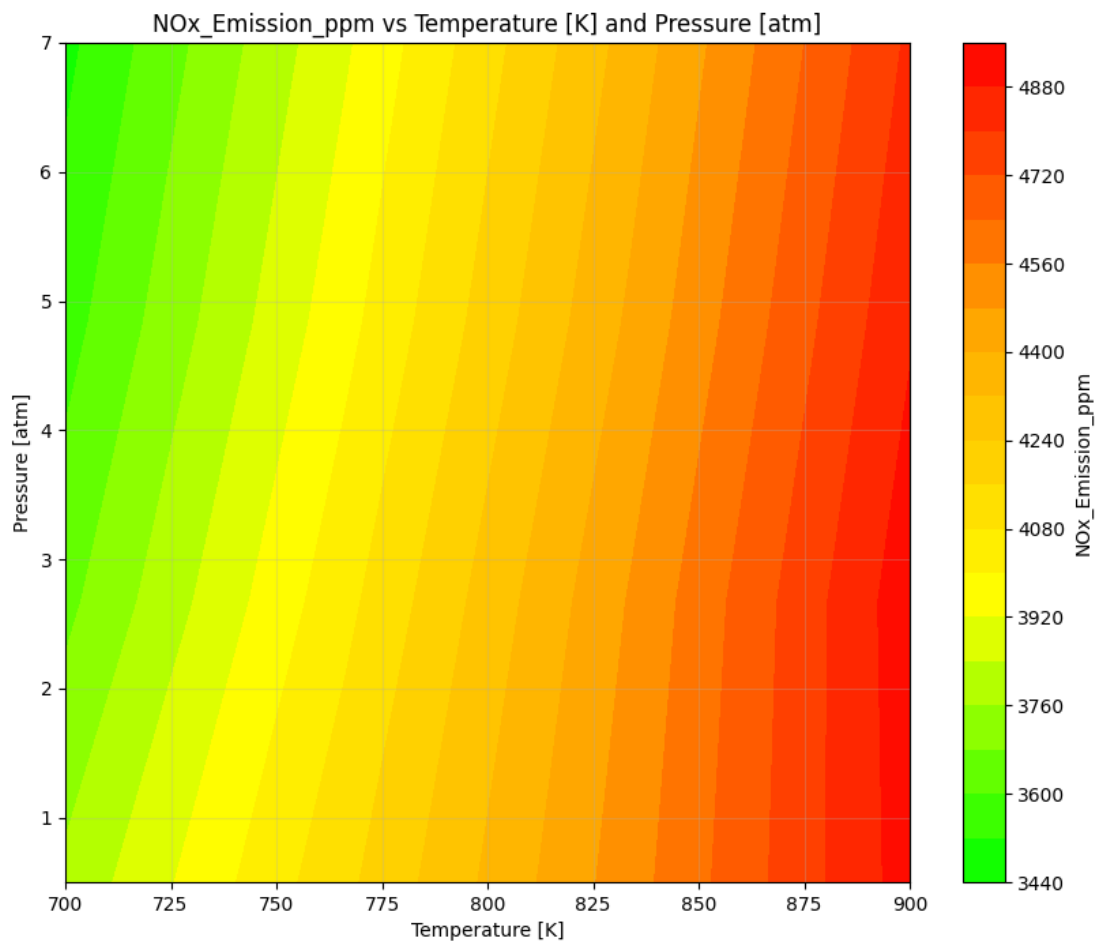
NOx emissions (ppm)

NOx\_Emission\_ppm vs Temperature [K] and Pressure [atm]



# Contour Plot: NOx\_Emission\_ppm

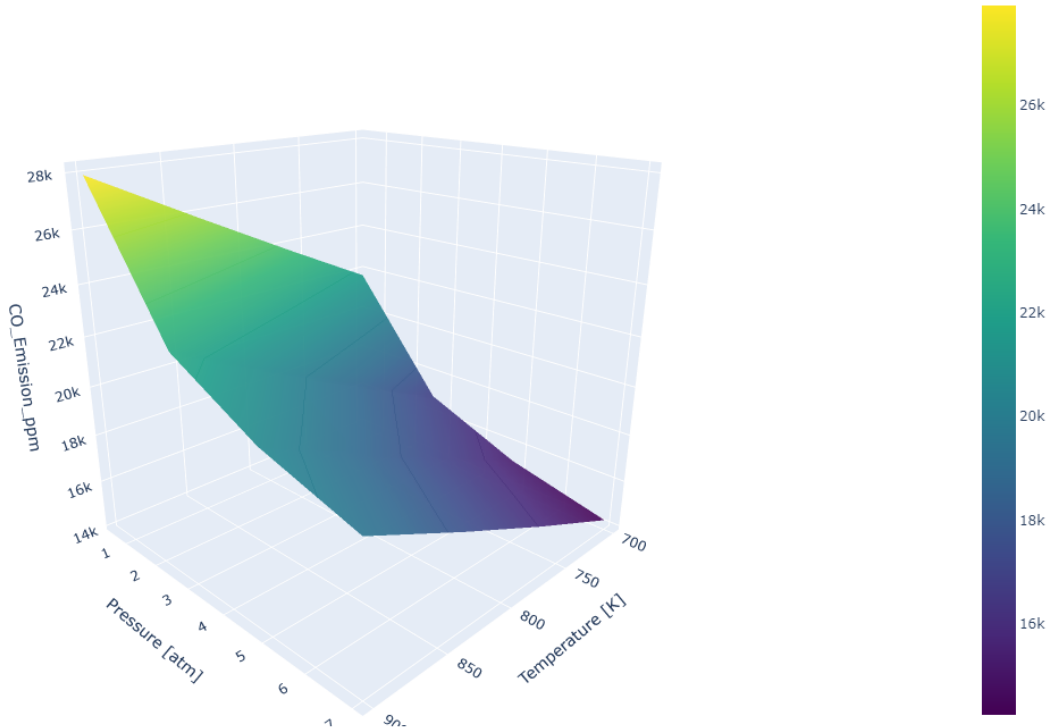
NOx emissions (ppm)



# 3D Plot: CO\_Emission\_ppm

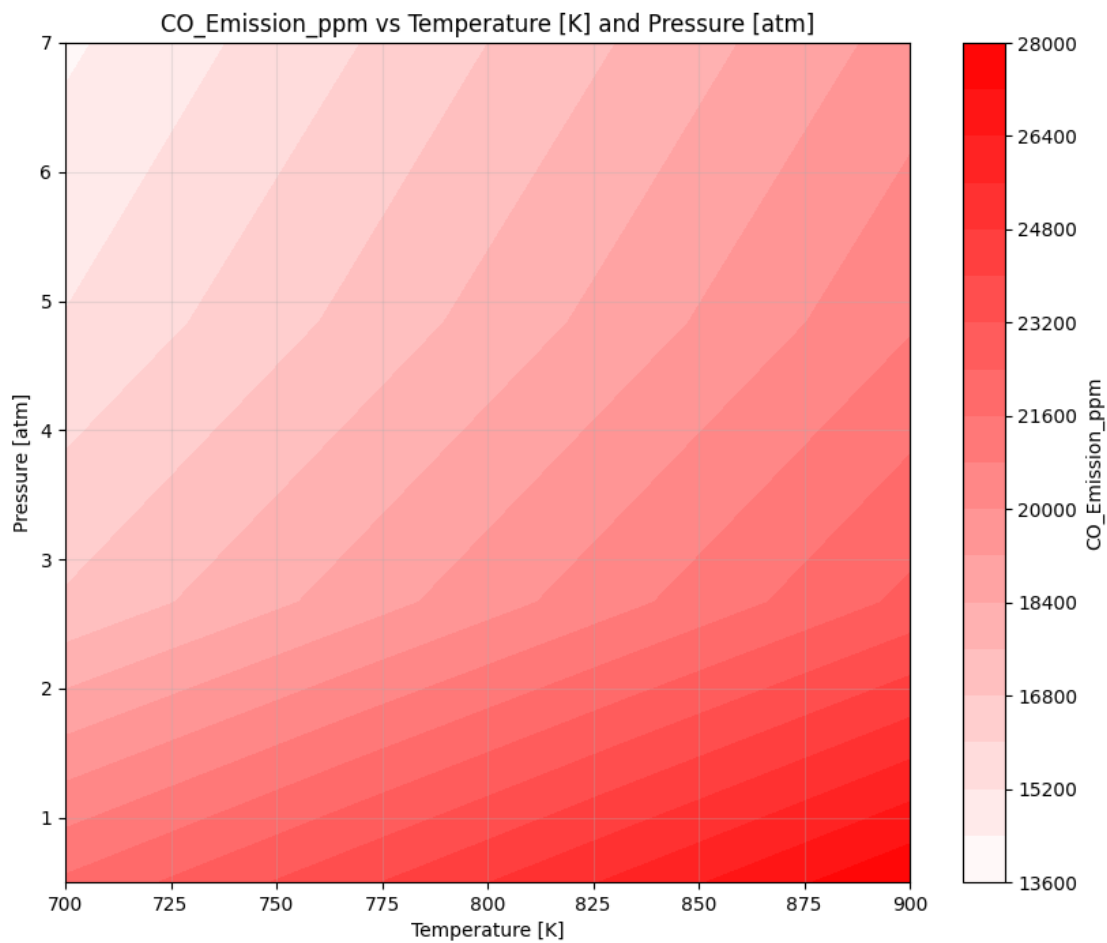
Carbon monoxide (CO) emissions (ppm)

CO\_Emission\_ppm vs Temperature [K] and Pressure [atm]



# Contour Plot: CO\_Emission\_ppm

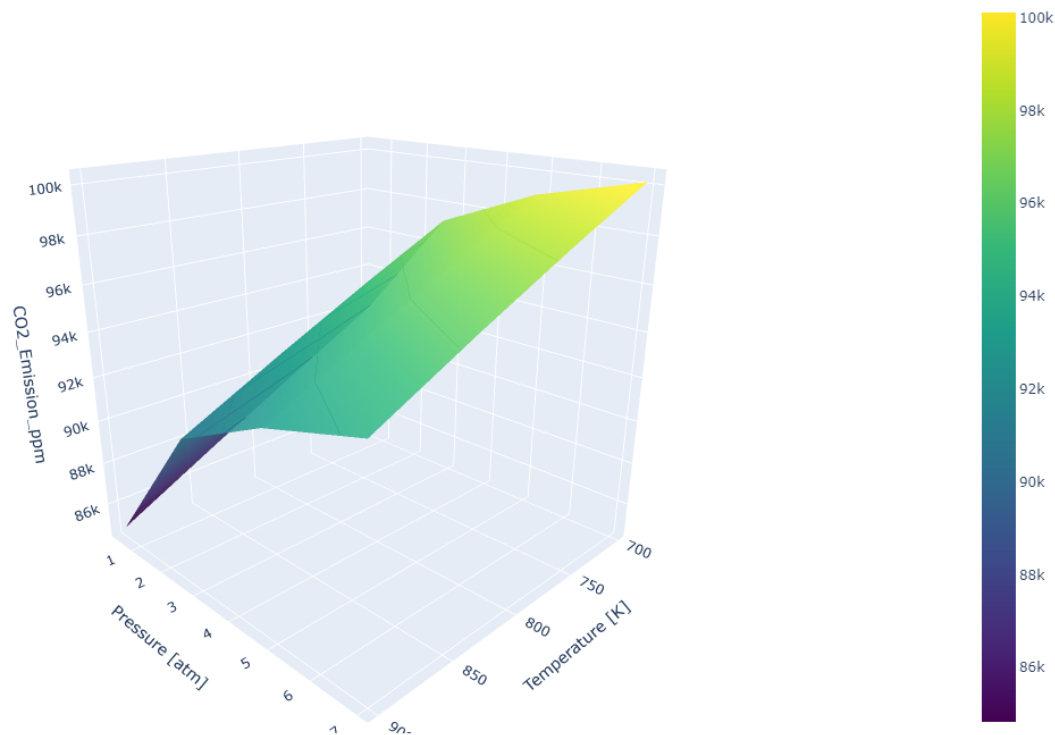
Carbon monoxide (CO) emissions (ppm)



# 3D Plot: CO2\_Emission\_ppm

Carbon dioxide (CO2) emissions (ppm)

CO2\_Emission\_ppm vs Temperature [K] and Pressure [atm]



# Contour Plot: CO2\_Emission\_ppm

Carbon dioxide (CO2) emissions (ppm)

