Overview of COMBI_BUMBI_v5

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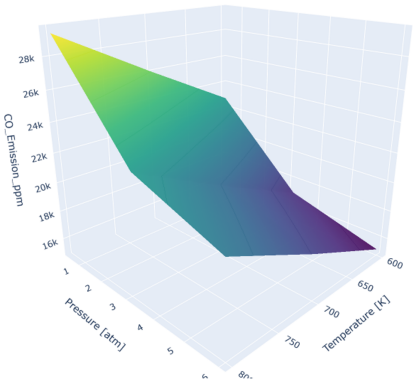
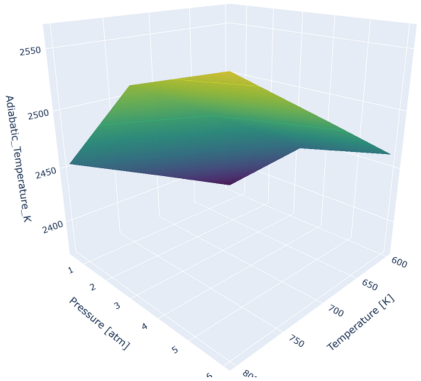
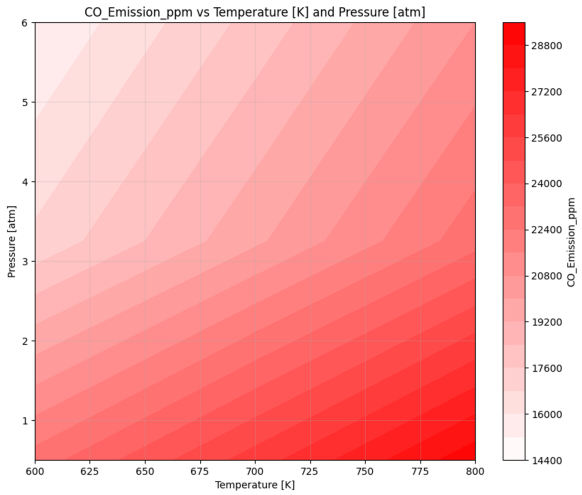
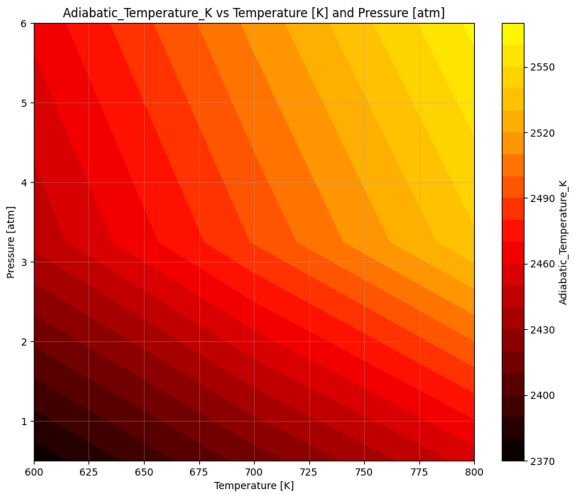








Contents

1 Introduction

The Combustion Parameters Analyzer (COMBI_BUMBI_v5) is a comprehensive graphical user interface (GUI) application designed for the analysis of combustion parameters across various fuels using Cantera.

COMBI_BUMBI_v5 supports a range of fuels including Hydrogen (H2), Methane (CH4), Carbon Monoxide (CO), Methanol (CH3OH) , Acetylene (C2H2), Ethylene (C2H4), Ethane (C2H6), Ammonia (NH3) [simplified], and Propane (C3H8). It also supports Air (21% O_2, 79% N_2), Oxygen (100% O_2), and Oxygen-Enriched Air (30% O_2) as oxidizers.

Key features of the application include multi-fuel and multi-oxidizer support , 3D surface visualizations (HTML + PNG) , contour plots with fuel-specific colormaps , advanced simulation parameter configuration , outlier compensation with adjustable thresholds , and automatic PDF report generation. Results provided by the application include adiabatic flame temperature, ignition delay time, laminar flame speed, NOx emissions, CO and CO_2 emissions (carbon-based fuels), a simulation settings summary, compensation records, and physical realism notes.

2 Requirements

To run COMBI_BUMBI_v5, the following software and Python packages are required:

2.1 Python

- Python 3.7 or higher

2.2 Python Packages

- `cantera >= 2.6.0`
- `numpy >= 1.20.0`
- `plotly >= 5.5.0`
- `matplotlib >= 3.4.0`
- `tkinter` (usually included with Python)
- `fpdf2 >= 1.7.6`
- `Pillow >= 9.0.0`
- `kaleido` (for plot export)

3 Calculation Methods

3.1 Adiabatic Flame Temperature (T_{ad})

- **Methodology:** The program initializes a Cantera gas mixture with the specified fuel, oxidizer, initial temperature (T), pressure (P), and equivalence ratio (ϕ). It then equilibrates this mixture at constant enthalpy and pressure ('HP') to determine the adiabatic flame temperature. This assumes a complete combustion process under ideal conditions where no heat is lost to the surroundings.
- **Cantera Object:** `gas_ad.equilibrate('HP')` is used on a copy of the initial gas state.

3.2 Ignition Delay Time

- **Methodology:** This parameter is calculated by simulating a constant-volume, adiabatic reactor using Cantera's `IdealGasReactor` and `ReactorNet`. The simulation progresses over time, recording temperature and, optionally, species concentrations.

- **Detection Methods:**
  - **Maximum Temperature Gradient (`max_dTdt`):** This is the default and robust general method. Ignition is detected at the point where the rate of temperature increase is highest.
  - **Maximum Concentration of Selected Intermediate Species (`max_species`):** This method detects ignition when the concentration of a specific intermediate radical (like OH, H, O, CO, or CH_2O) reaches its peak. The user can select the species to monitor, with recommendations provided for different fuel types and combustion conditions.
- **Advanced Settings:**
  - **Simulation End Time (`ignition_end_time`):** Defines the maximum duration for the ignition delay simulation. If ignition doesn't occur within this time, the delay is reported as 0.0 or the end time.
  - **Temperature Threshold (`ignition_temp_threshold`):** Sets the minimum temperature rise from the initial temperature required to consider ignition.
- **Unit:** The ignition delay is returned in microseconds (μs).

3.3 Laminar Flame Propagation Speed

- **Methodology:** The program calculates the laminar flame speed using Cantera's `FreeFlame` model. This involves solving for the one-dimensional, steady-state flame structure.
- **Advanced Settings:**
  - **Flame Width (`flame_width`):** This parameter sets the initial domain width for the calculation, defining the spatial extent over which the flame structure is determined. An appropriate width is crucial for solver convergence.
- **Solver Stability:** The code includes improved solver stability settings like `set_refine_criteria` and `set_max_jac_age` for robust calculations.
- **Unit:** The laminar flame speed is returned in meters per second (m/s).

3.4 Emissions (NOx, CO, CO_2)

- **Methodology:** Emissions of Nitric Oxide (NOx), Carbon Monoxide (CO), and Carbon Dioxide (CO_2) are determined from the species concentrations in the adiabatic equilibrium products (calculated for adiabatic flame temperature).

3.5 Specific Reaction Mechanisms

The program leverages different Cantera reaction mechanisms (`.yaml` files) based on the selected fuel to accurately model the chemical reactions during combustion:

- **`h2o2.yaml`:** This mechanism is specifically used when Hydrogen (H_2) is selected as the fuel. The `h2o2.yaml` mechanism is suitable for simulating hydrogen-oxygen combustion systems, including the formation of water and the key radical species involved.
- **`gri30.yaml`:** This is a widely used and comprehensive mechanism employed when Methane (CH_4) and other hydrocarbon fuels are selected. The GRI-Mech 3.0 mechanism includes detailed reaction pathways for methane and natural gas combustion, covering a broad range of species and conditions relevant to hydrocarbon flames.

4 Graphical User Interface (GUI)

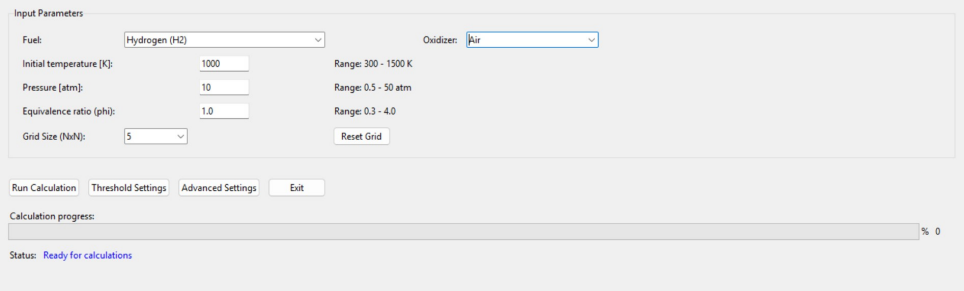


Figure 1: Main page of the COMBI_BUMBI_v5 GUI

The `COMBI_BUMBI_v5` program features a user-friendly Graphical User Interface (GUI), with its main page allowing users to configure various combustion parameters.

Key sections and selectable options include:

4.1 Fuel Selection

The application offers a selection of nine distinct fuels for analysis:

- Hydrogen (H_2)
- Carbon Monoxide (CO)
- Methanol (CH_3OH)
- Acetylene (C_2H_2)
- Ethylene (C_2H_4)
- Ethane (C_2H_6)
- Ammonia (NH_3)
- Propane (C_3H_8)

4.2 Oxidizer Selection

Users can choose from three types of oxidizers:

- Air (21% O_2; 79% N_2)
- Oxygen Enriched Air (30% O_2)
- Pure Oxygen (100% O_2)

4.3 Initial Parameters

Essential initial conditions for the combustion analysis can be specified:

- **Temperature:** Must be provided within the range of 300 K to 1500 K.
- **Pressure:** Must be provided within the range of 0.5 atm to 50 atm.
- **Equivalence Ratio:** Must be provided within the range of 0.3 to 4.

4.4 Grid Size

Recognizing that calculations can be computationally intensive, `COMBI_BUMBI_v5` allows users to select the grid resolution, ranging from 2x2 to 10x10. Smaller grid resolutions (e.g., 2x2 or 3x3) typically complete calculations within approximately 5 minutes, while larger resolutions (e.g., 10x10) may require several hours. Generally, more complex fuels (those with a higher number of atoms) necessitate longer calculation times. Adjacent to the grid resolution selector, a "Reset Grid" button is available to revert the resolution to its default value of 5x5.

4.5 Progress Bar

This element provides the user with real-time information regarding the calculation status of grid points. Upon completion of all grid point calculations, the bar then transitions to display the progress of plot and report generation.

Figure 2: The progress bar displaying calculations of grid points.

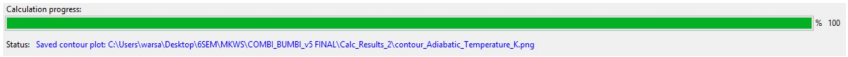


Figure 3: The progress bar indicating progress during plot and report generation.

5 Threshold Settings

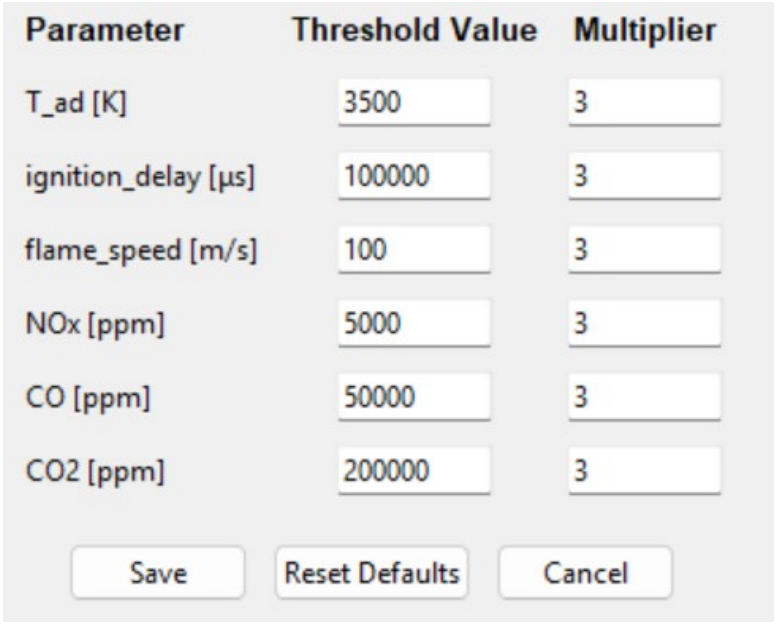


Figure 4: Threshold Settings Panel

An outlier compensation mechanism identifies and adjusts extreme or potentially erroneous calculated values. These thresholds work with specific multipliers to modify values deemed outliers. There are six such threshold settings, each corresponding to a combustion parameter:

- `temp_threshold`: For Adiabatic Flame Temperature (T_{ad})
- `nox_threshold`: For NOx emissions
- `co_threshold`: For CO emissions
- `co2_threshold`: For CO2 emissions
- `speed_threshold`: For Laminar Flame Speed
- `ignition_threshold`: For Ignition Delay Time

5.1 How These Threshold Settings Work:

- **Detection**: Each threshold (e.g., `temp_threshold` set at 3500 K) represents an upper limit. If a calculated value for its respective parameter (e.g., a calculated T_{ad}) exceeds this predefined threshold, it is flagged as an outlier.
- **Compensation**: Once a value is identified as an outlier, the program attempts to compensate for it. The method involves:
  - Calculating the median of the "good" (non-outlier) surrounding data points for that specific parameter.
  - Multiplying this median by a predetermined multiplier (e.g., `temp_multiplier`, `nox_multiplier`, etc.). In the provided program's default configuration, these multipliers are typically set to 3, meaning the adjusted value will be 3 times higher than the median of the surrounding points.
  - The outlier value is then replaced with this adjusted median-based value.

This mechanism helps smooth out and correct values that might be unrealistically high due to computational artifacts or other issues, ensuring more robust and consistent results.

5.2 Upon saving the threshold settings, a confirmation message will be displayed below the progress bar:

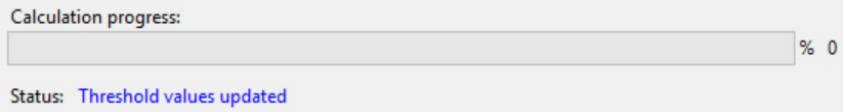


Figure 5: Displayed confirmation message

6 Advanced Simulation Parameter Configuration

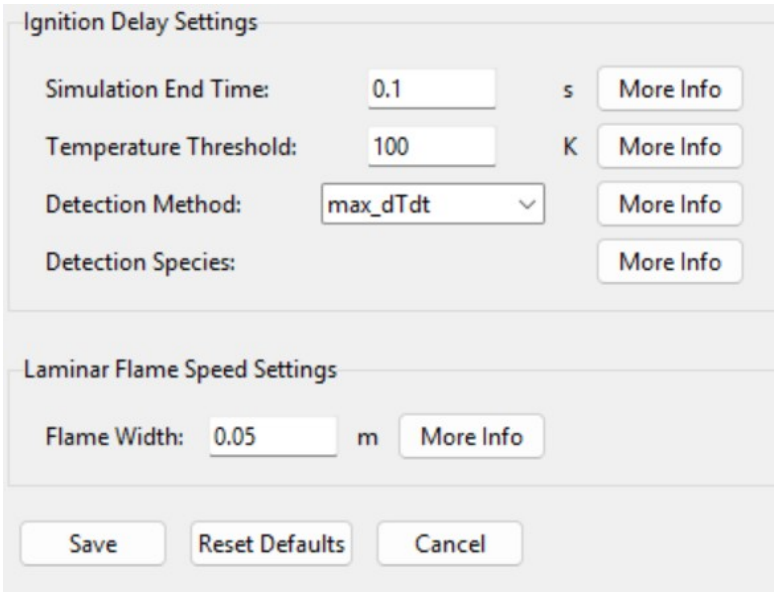


Figure 6: Advanced settings Panel

The Combustion Parameters Analyzer (COMBI BUMBI_v5) offers an "Advanced Settings" interface, providing users with precise control over the underlying simulation parameters. These settings specifically impact the computational engine (Cantera) for **Ignition Delay** and **Laminar Flame Speed** calculations, enabling tailored and robust analysis for diverse fuel and oxidant combinations.

6.1 Functionality

The `AdvancedSettingsDialog` class manages these parameters via a dedicated graphical user interface (GUI).

- **Loading and Modification:** Upon opening the dialog, the current advanced settings are loaded. Users can modify these values, which are then stored within the application's `advanced_settings` attribute upon saving.
- **Simulation Impact:** The updated settings are subsequently utilized during combustion calculations, directly influencing the simulation behavior for both ignition delay and flame speed. **User Guidance:** Each setting includes "More Info" buttons, offering detailed descriptions to aid user understanding.
- **Default Restoration:** A "Reset Defaults" button allows for the restoration of all advanced settings to their predefined original values.

6.2 Configurable Parameters

6.2.1 Ignition Delay Settings

- **Simulation End Time (`ignition_end_time`):**
  - **Purpose**: Defines the maximum duration for the ignition delay calculation. If ignition is not detected within this period, the delay is reported as 0.0 or the end time.
  - **Guidance**: Increase this value for slow ignitions (e.g., low temperatures/pressures, less reactive fuels). A positive value is required. Excessive values will significantly increase calculation time.

- **Temperature Threshold (`ignition_temp_threshold`)**:
  - **Purpose**: Specifies the minimum temperature increase from the initial temperature required to detect ignition.
  - **Guidance**: A higher value enhances robustness against numerical fluctuations. A smaller value may detect weaker ignitions but could be triggered by noise. The default is 100 Kelvin. A positive value is required.
- **Detection Method (`ignition_detection_method`)**:
  - **Purpose**: Determines the methodology for identifying ignition delay.
  - **Options**:
    - **Maximum Temperature Gradient (max_dTdt)**: A robust, general-purpose method that detects ignition at the point of maximum temperature increase rate.
    - **Maximum Concentration of Selected Intermediate Species (max_species)**: Detects ignition when a specified intermediate radical (e.g. OH, H, O) reaches its peak concentration. This method can offer greater sensitivity for specific fuels or conditions.
  - **Recommendation**: "max_dTdt" is recommended for general applications. "max_species" is suitable when a specific radical is known to be a strong indicator for the fuel under consideration.
- **Detection Species (`ignition_detection_species`)**:
  - **Purpose**: Specifies the intermediate species to be monitored for ignition delay when the "max_species" method is selected. **This option becomes available for selection *only after* "Maximum Concentration of Selected Intermediate Species (max_species)" is chosen as the `Detection Method`.**
  - **Options**: OH, H, O, CO, CH2O.

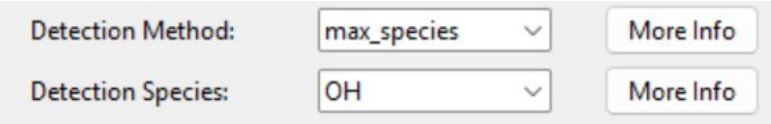


Figure 7: The **species selection panel**, displayed following the selection of the `max_species` detection method.

  - **Recommendations**:
    - **OH, H, O**: Common, highly reactive radicals suitable for most hydrocarbon fuels and hydrogen. OH is frequently preferred for general hydrocarbon combustion.
    - **CO (Carbon Monoxide)**: Relevant if CO formation is a critical indicator, particularly for fuels exhibiting early CO production.
    - **CH2O (Formaldehyde)**: Important for low-temperature combustion of alkanes; consider for larger alkanes (e.g., Propane) at lower initial temperatures where cool flames may precede hot ignition.

6.2.2 Laminar Flame Speed Settings

- **Flame Width (`flame_width`)**:
  - **Purpose**: Sets the initial spatial domain for laminar flame speed calculations.
  - **Guidance**: A larger width may be necessary for thick flames or very low pressures, though it increases computation time. A smaller width might prevent convergence. The default is 0.05m (5 cm). A positive value is required. Increasing this value can assist if the solver fails to converge.

6.3 Purpose of Advanced Settings

These advanced settings are instrumental for tailoring the simulation to accurately model combustion phenomena across varying conditions and fuel types. They empower users to:

- **Enhance Accuracy**: Refine the precision of ignition delay calculations by adjusting temperature thresholds and detection methods.
- **Optimize Performance**: Balance computational efficiency with simulation depth by modifying `ignition_end_time` and `flame_width`.
- **Specialize Analysis**: Adapt the simulation to specific fuel characteristics or operating conditions by selecting the appropriate `ignition_detection_species` or method.
- **Address Convergence Issues**: Overcome numerical challenges, such as non-convergence in laminar flame speed calculations, by adjusting parameters like `flame_width`.

In summary, the Advanced Settings enable expert users to precisely control the intricate aspects of combustion simulations, thereby ensuring scientifically sound and highly relevant results for their analytical or research objectives.

7 Fallback Features

The `COMBI_BUMBI_v5.txt` file describes several fallback features and error handling mechanisms within its combustion parameter calculation routines, particularly for ignition delay and, to a lesser extent, other calculations.

7.1 Fallback Features in Ignition Delay Calculation:

The system offers robust handling for ignition delay calculations, including:

- **Maximum Simulation Time (`ignition_end_time`)**: A maximum simulation time is set for ignition delay calculations. If ignition does not occur within this specified duration, the ignition delay is reported as 0.0 or the `end_time` itself. This prevents calculations from running indefinitely for non-igniting conditions. This setting can be increased for slower ignitions (e.g., at low temperatures or pressures).
- **Species Availability Fallback**: If the user selects the `max_species` detection method and the chosen detection species (e.g., 'OH', 'H', 'O', 'CO', 'CH2O') is not found within the loaded chemical mechanism (e.g., `h2o2.yaml`, `gri30.yaml`), the system automatically falls back to the `max_dTdt` method for that specific ignition delay calculation. A warning is logged when this switch occurs.
- **Insufficient Data Handling**: In cases where there is insufficient data (e.g., very few time steps) or no significant temperature rise observed during the simulation, the ignition delay is set to 0.0. This also serves as a fallback if the `max_species` method fails or provides bad data, prompting a default to `max_dTdt` if enough temperature data is available.

7.2 Fallback/Error Handling in Other Calculations:

- **Laminar Flame Speed Calculation (`flame_width`)**: For laminar flame speed calculations, an initial domain width (`flame_width`) is set. If the flame solver fails to converge, the description advises increasing this value, indicating a user-driven adjustment for solver stability rather than an automatic fallback within the code. If the flame solver fails or yields a non-positive velocity, the flame speed is set to 0.0.
- **General Calculation Error Handling**: The main `run_calculation` function includes a broad `try-except` block. If any general exception occurs during the overall calculation process, an error message is displayed to the user and logged. In such cases, all calculated results are set to 0. This acts as a generalized error handling mechanism to prevent the program from crashing, although it does not involve alternative calculation methodologies.

8 Running the Program

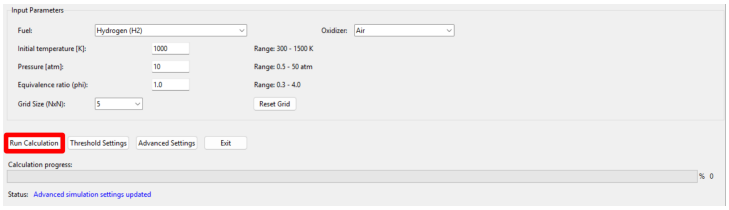


Figure 8: Main Graphical User Interface (GUI) page, highlighting the `Run Calculation` button.

Initiating a calculation within the program is performed by clicking the **"Run Calculation"** button. Users are advised to await the appearance of a "Success" pop-up notification, which confirms the successful completion of the calculation process.

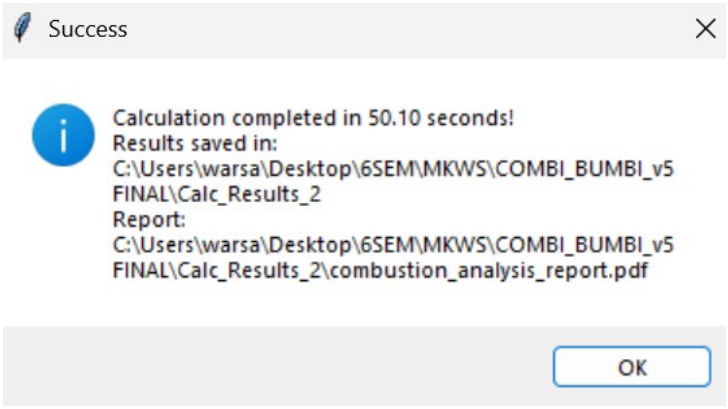


Figure 9: Success pop-up window

Upon completion of a calculation, the program automatically generates a dedicated results directory. This directory, named `Calc_Results_X` (where X is an incrementing integer, e.g., `Calc_Results_2` if `Calc_Results` and `Calc_Results_1` already exist), is created in the same location as the `COMBI_BUMBI_v5.py` executable.

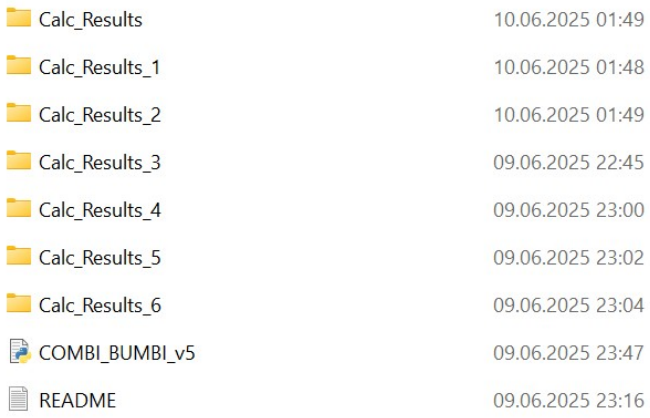


Figure 10: Example of the `Calc_Results` folder naming convention within the directory containing the `COMBI_BUMBI_v5.py` executable.

All generated data and reports are systematically saved within the aforementioned `Calc_Results_X` folder. The contents include:

- **Log file**
  - `log (TXT)`
- **HTML 3D plots**
  - `3d_plot_Adiabatic_Temperature_K (HTML)`
  - `3d_plot_CO_Emission_ppm (HTML)` (Generated only for fuels containing carbon)
  - `3d_plot_CO2_Emission_ppm (HTML)` (Generated only for fuels containing carbon)
  - `3d_plot_Flame_Speed_m_s (HTML)`
  - `3d_plot_Ignition_Delay_us (HTML)`
  - `3d_plot_NOx_Emission_ppm (HTML)`
- **HTML 3D plots screenshots**
  - `3d_plot_Adiabatic_Temperature_K (PNG)`
  - `3d_plot_CO_Emission_ppm (PNG)` (Generated only for fuels containing carbon)
  - `3d_plot_CO2_Emission_ppm (PNG)` (Generated only for fuels containing carbon)
  - `3d_plot_Flame_Speed_m_s (PNG)`
  - `3d_plot_Ignition_Delay_us (PNG)`
  - `3d_plot_NOx_Emission_ppm (PNG)`
- **PNG contour Plots**
  - `contour_CO_Emission_ppm (PNG)` (Generated only for fuels containing carbon)
  - `contour_CO2_Emission_ppm (PNG)` (Generated only for fuels containing carbon)
  - `contour_Flame_Speed_m_s (PNG)`
  - `contour_Ignition_Delay_us (PNG)`
  - `contour_NOx_Emission_ppm (PNG)`
  - `contour_Adiabatic_Temperature_K (PNG)`
- **PDF Report**
  - `combustion_analysis_report (PDF)`

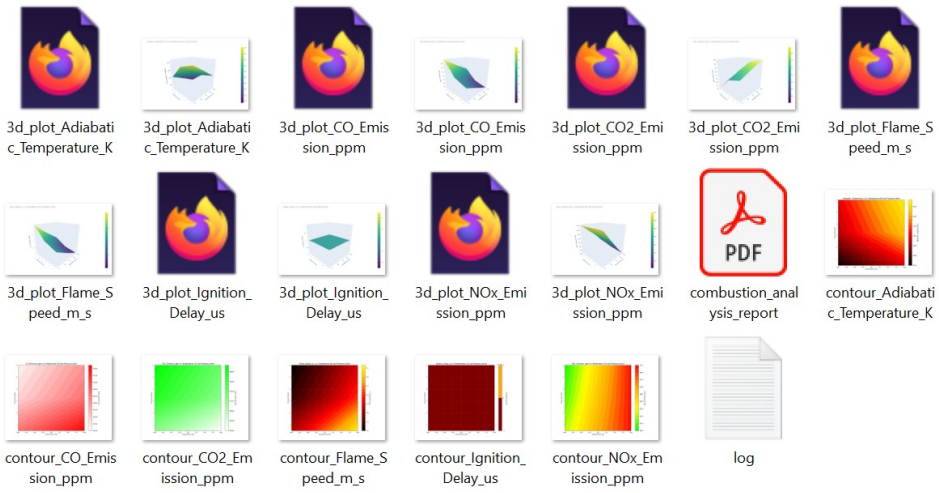


Figure 11: Example of file saved inside `Calc_Results` folder

9 Logging

The log file captures various types of messages, categorized by their severity:

- **Informational Messages (`logging.info`)**: These messages provide general information about the application's progress and significant events. Examples include:
  - Confirmation of logging setup and the path to the log file.
  - Details about loaded chemical mechanisms (e.g., `gri30.yaml`).
  - Start and end times of calculations.
  - Parameters used for simulations (e.g., pressure, temperature, equivalence ratio).
  - Confirmation of successful data plotting or PDF generation.
- **Warning Messages (`logging.warning`)**: These messages indicate potential issues or non-critical errors that the application handled but might warrant user attention. A significant example from the provided code is:
  - Warnings when a specified ignition detection species (e.g., 'OH', 'H', 'O') is not found in the loaded Cantera mechanism, leading to an automatic fallback to the "Maximum Temperature Gradient" method for ignition delay calculation.
  - Warnings related to failed convergence for certain calculations, or issues with output file generation.
- **Error Messages (`logging.error`)**: These messages signify more severe problems that prevented a specific operation from completing successfully. Examples include:
  - Errors encountered during the calculation process (e.g., Cantera simulation failures, mathematical errors).
  - Issues with file operations, such as failing to load a chemical mechanism or an image for PDF generation.
  - General exceptions caught within `try-except` blocks that handle unexpected program behavior.

9.1 Specific Events and Data Logged:

- **Initialization and Configuration**:
  - The setup of the logging system itself, including the path where the log file is being written.
  - Details about the Cantera mechanism (`.yaml` file) being loaded, including any potential issues during loading.
- **Simulation Parameters**:
  - The initial conditions for various simulations, such as pressure, temperature, equivalence ratio, and fuel composition.
  - Advanced settings used for ignition delay calculation, like `ignition_end_time`, `ignition_temp_threshold`, `ignition_detection_method`, and `ignition_detection_species`.
  - Settings for laminar flame speed calculations, such as `flame_width`.
- **Calculation Progress and Results**:
  - Status updates indicating the start and completion of different calculation types (e.g., ignition delay sweep, flame speed calculation, adiabatic flame temperature).
  - Warnings or errors if a calculation fails to converge or produces invalid results (e.g., negative flame speed).
  - Information about the detection method used for ignition delay, especially when a fallback occurs switching method to `max_dTdt`.
  - Information about outlier compensation and threshold adjustments.

- **Output Generation**:
  - Confirmation messages when plots are generated and saved to files (e.g., `ignition_delay_plot.html`, `flame_speed_plot.html`).
  - Messages related to the creation of the results PDF report, including any errors encountered during image loading or PDF generation.
- **Error Details**:
  - Tracebacks for exceptions caught during program execution, providing detailed information about where and why an error occurred. This is crucial for debugging.

```
2025-06-15 20:00:37,544 - WARNING - Selected species 'CO' not found in mechanism 'h2o2.yaml'. Switching to max_dTdt for ignition delay.
2025-06-15 20:00:37,544 - INFO - No significant temperature rise or insufficient data for ignition for T=900.0K, P=5.0atm, phi=1.0. Setting ignition delay
to 0.0.
2025-06-15 20:00:38,679 - WARNING - Flame solver failed for T=1000.0K, P=5.0atm, phi=1.0: index 8 is out of bounds for axis 0 with size 8. Attempting with
different initial guess or width.
2025-06-15 20:00:48,140 - WARNING - Flame speed calculation yielded non-positive velocity for T=1000.0K, P=10.0atm, phi=1.0. Setting to 0.0.
```

Figure 12: Illustrative example of entries within the `log.txt` file.

10 HTML 3D plots

The COMBI BUMBI_v5 application produces 3D surface visualizations in HTML format, encompassing various combustion parameters:

- Adiabatic Flame Temperature (K)
- CO Emission (ppm) (generated exclusively for carbon-based fuels)
- CO2 Emission (ppm) (generated exclusively for carbon-based fuels)
- Flame Speed (m/s)
- Ignition Delay (μs)
- NOx Emission (ppm)

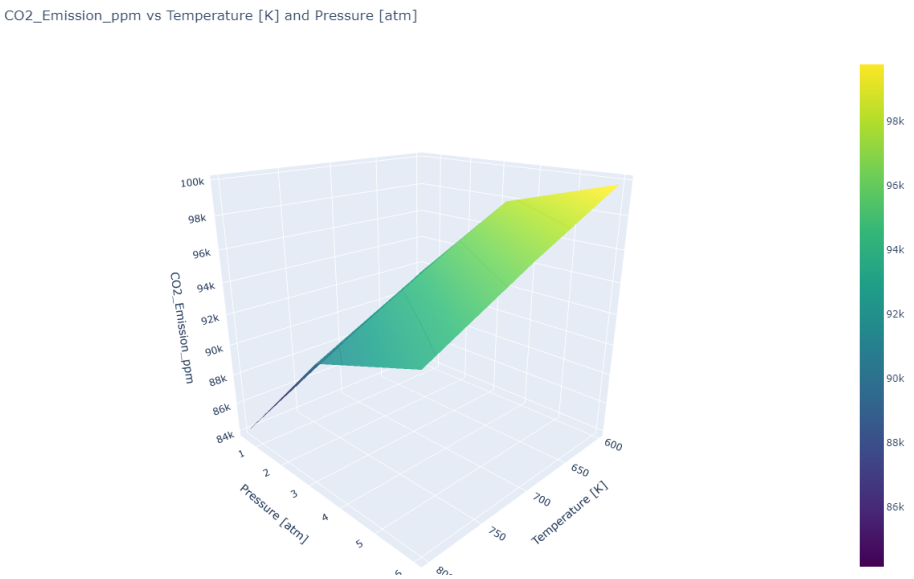


Figure 13: Representative 3D HTML plot, specifically illustrating `3d_plot_CO2_Emission_ppm.png`

These interactive HTML plots are located within the `Calc_Results_X` directory, which is automatically generated in the same directory as the `COMBI_BUMBI_v5.py` executable. Users can access these visualizations by opening the respective HTML files (e.g., `3d_plot_Adiabatic_Temperature K (HTML)`) directly with a web browser. Furthermore, corresponding PNG screenshots of these 3D HTML plots are also provided.

11 Contour Plots

The $\mathrm{COMBI}_{BUMBI_v5 application produces 3D surface visualizations, which can be represented as contour plots, encompas$

- Adiabatic Flame Temperature (K)
- CO Emission (ppm) (generated exclusively for carbon-based fuels)
- CO2 Emission (ppm) (generated exclusively for carbon-based fuels)
- Flame Speed (m/s)
- Ignition Delay (μs)
- NOx Emission (ppm)

These plots visualize the calculated parameters across a range of initial temperatures and pressures.

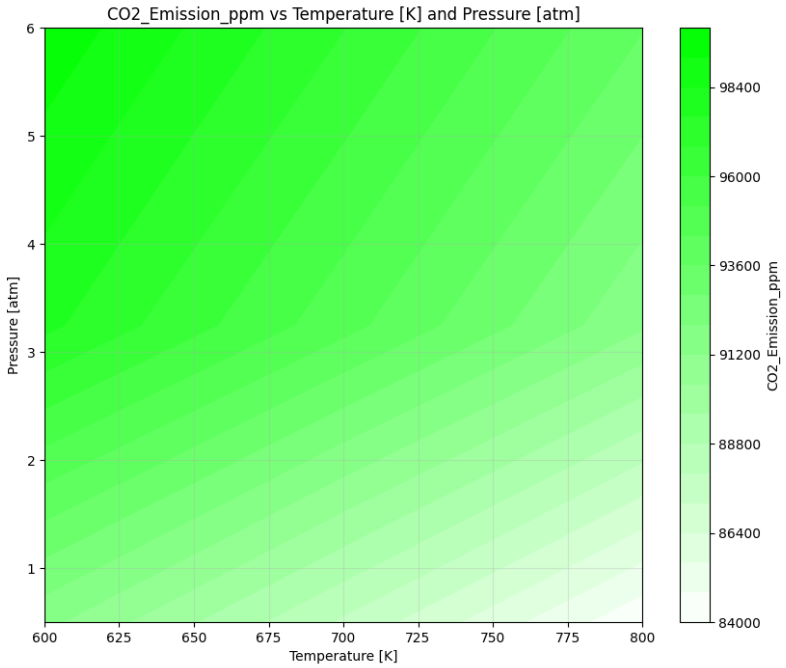


Figure 14: Representative contour plot, specifically illustrating `contour_CO2_Emissio_ppm.png`

12 Combustion Analysis Report (PDF Report)

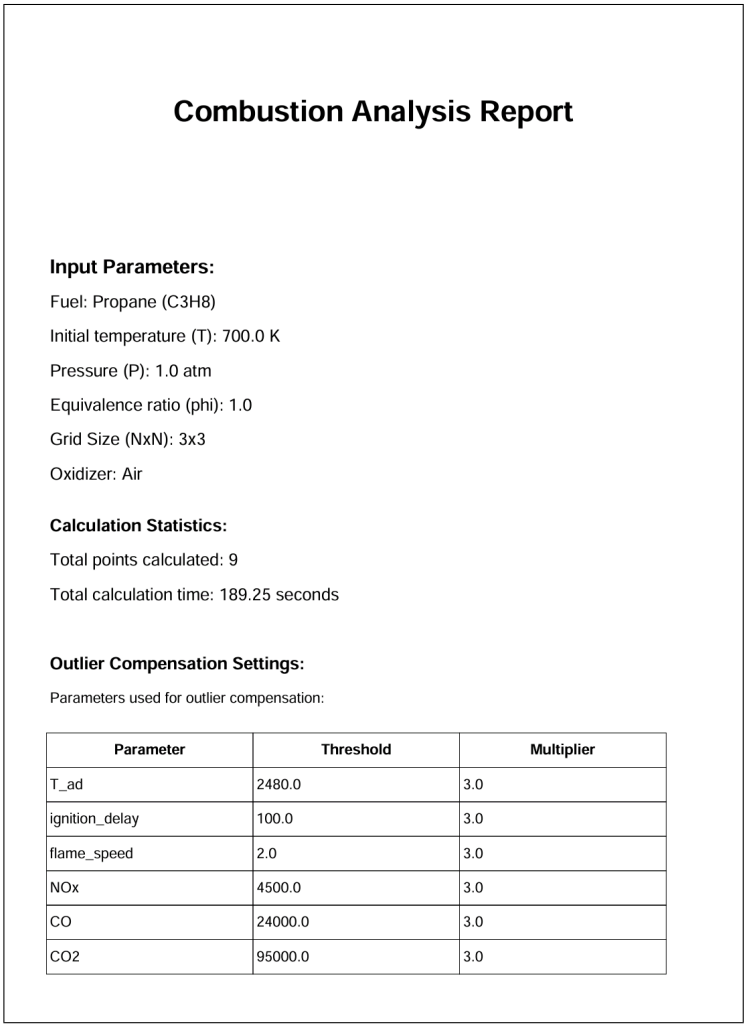
The Combustion Analysis Report provides a comprehensive overview of combustion parameters for propane (C3H8) fuel with air as the oxidizer. The report details input parameters, calculation statistics, and outlier compensation settings, including thresholds and multipliers for various parameters like adiabatic temperature, ignition delay, flame speed, NOx, CO, and CO2 emissions. It also outlines advanced simulation settings, such as ignition end time, temperature threshold, and flame width.

The report includes a section on compensated data points, listing original and adjusted values for adiabatic temperature, flame speed, and NOx emissions at specific temperatures and pressures. Important notes on physical realism are provided, discussing the interpretation of ignition delay, NOx, CO, CO2 emissions, and flame speed plots, along with general interpretation guidelines and warnings about result reliability at extreme conditions.

Visualizations are presented through 3D plots and contour plots for key combustion parameters:

- Adiabatic Temperature (K)
- Ignition Delay (μs)
- Flame Speed (m/s)
- NOx Emissions (ppm)
- CO Emissions (ppm) (Generated only for fuels containing carbon)
- CO2 Emissions (ppm) (Generated only for fuels containing carbon)

The report also specifies the generation date and the directory where the results are stored.



Combustion Analysis Report

Input Parameters:

Fuel: Propane (C3H8)

Initial temperature (T): 700.0 K

Pressure (P): 1.0 atm

Equivalence ratio (phi): 1.0

Grid Size (NxN): 3x3

Oxidizer: Air

Calculation Statistics:

Total points calculated: 9

Total calculation time: 189.25 seconds

Outlier Compensation Settings:

Parameters used for outlier compensation:

Parameter	Threshold	Multiplier
T_ad	2480.0	3.0
ignition_delay	100.0	3.0
flame_speed	2.0	3.0
NOx	4500.0	3.0
CO	24000.0	3.0
CO2	95000.0	3.0

Figure 15: Representative Front Page of a `Combustion Analysis Report`.

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

Generated: 2025-06-15 22:57:15

Results directory: C:\Users\warsa\Desktop\6SEM\MKWS\COMBI_BUMBI_v5 F\Calc_Results

Figure 16: Representative Second Page of a `Combustion Analysis Report`.

Compensated Data Points

T_ad at T=700.0K, P=3.25atm: Original value 2491 was compensated to 2480 (Extreme value (2.49e+03))

T_ad at T=800.0K, P=3.25atm: Original value 2538 was compensated to 2480 (Extreme value (2.54e+03))

T_ad at T=700.0K, P=6.0atm: Original value 2513 was compensated to 2480 (Extreme value (2.51e+03))

flame_speed at T=700.0K, P=0.5atm: Original value 2.383 was compensated to 2 (Extreme value (2.38e+00))

flame_speed at T=800.0K, P=0.5atm: Original value 3.108 was compensated to 2 (Extreme value (3.11e+00))

flame_speed at T=800.0K, P=3.25atm: Original value 2.259 was compensated to 2 (Extreme value (2.26e+00))

NOx at T=700.0K, P=0.5atm: Original value 4506 was compensated to 4500 (Extreme value (4.51e+03))

NOx at T=800.0K, P=0.5atm: Original value 5125 was compensated to 4500 (Extreme value (5.13e+03))

NOx at T=800.0K, P=3.25atm: Original value 5088 was compensated to 4500 (Extreme value (5.09e+03))

NOx at T=800.0K, P=6.0atm: Original value 4999 was compensated to 4500 (Extreme value (5.00e+03))

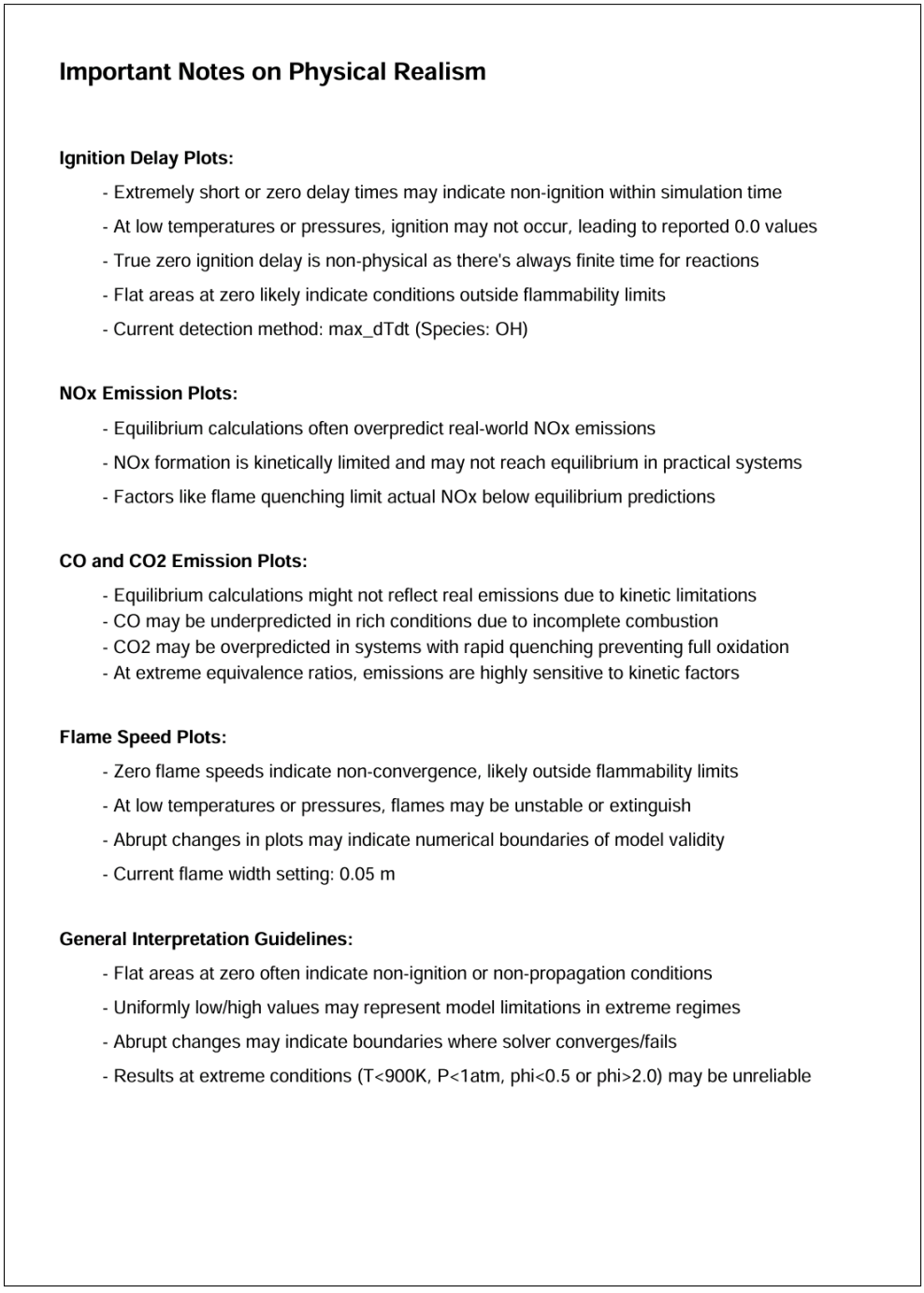
CO at T=700.0K, P=0.5atm: Original value 2.598e+04 was compensated to 2.4e+04 (Extreme value (2.60e+04))

CO at T=800.0K, P=0.5atm: Original value 2.934e+04 was compensated to 2.4e+04 (Extreme value (2.93e+04))

CO2 at T=600.0K, P=3.25atm: Original value 9.781e+04 was compensated to 9.5e+04 (Extreme value (9.78e+04))

CO2 at T=600.0K, P=6.0atm: Original value 9.976e+04 was compensated to 9.5e+04 (Extreme value (9.98e+04))

Figure 17: Exemplar page from a `Combustion Analysis Report`, depicting Compensated Data Points determined by `Threshold settings`.



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<900K, P<1atm, phi<0.5 or phi>2.0) may be unreliable

Figure 18: Exemplar page from a `Combustion Analysis Report`, illustrating the `Important Notes on Physical Realism` section.

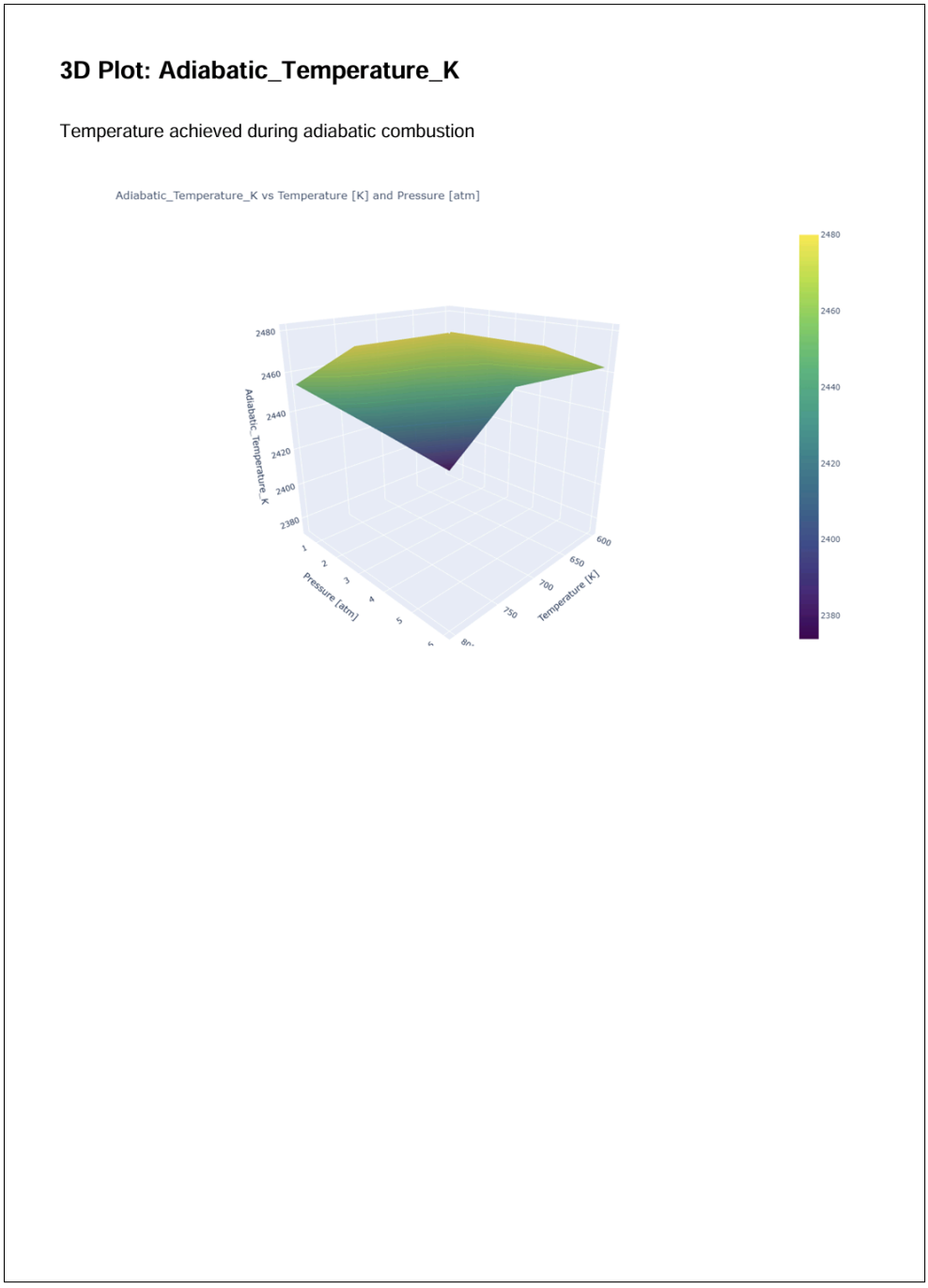


Figure 19: Exemplar page from a `Combustion Analysis Report`, displaying the `3D HTML Adiabatic_Temperature plot`.