CONTROLLING SOFTWARE AND OPTIMIZATION FOR COMPRESSOR ENGINE'S OPERATION UNDER VARIABLE GAS COMPOSITION

An Undergraduate Research Scholars Thesis

by

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ABSTRACT

Controlling Software and Optimization for Compressor Engine's Operation Under Variable Gas Composition

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This research will determine what controller type and code must be implemented to ensure the operation of a natural gas compressor station engine stays within emission standards. The natural gas pipeline compressor stations power the transportation of extracted natural gas downstream. The engines that power these stations run off the natural gas being fed through the line. As fracking occurs to extract natural gas, the newly accessed natural gas deposits do not have a single level of chemical composition, as they would have in a natural gas reservoir. Thus, the engines that are fed the natural gas from areas that utilize techniques such as fracking must be able to adapt their operation to still run to meet emission standards and continue to move the natural gas. The controller to be designed must run the compressor station engines to meet emission standards and still provide enough power to pass the natural gas along the pipeline.

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NOMENCLATURE

HHV	Higher Heating Value
NOx	Nitrous Oxides
WI	Wobbe Index
SG	Specific Gravity
LHV	Lower Heating Value
PID	Proportional integral derivative
TDC	Top Dead Center
BDC	Bottom Dead Center
MPC	Model Predictive Control

CHAPTER I

INTRODUCTION

When natural gas is extracted from the ground, the chemical composition of the gas can vary over a period of time "as short as a few minutes to periods of several days due to formations containing increased heavy hydrocarbons or inert contents."[1] The development of natural gas production within the United States has only increased the focused on fracking to extract the trapped gasses within scattered shale pockets. Since natural gas has various stable chemical forms, the gas within each well reaches different chemical equilibrium conditions in multiple sections, inherently causing variance of the gas being extracted. Furthermore, the gas is transported along a pipeline that connects to multiple sources. This network of sources into the pipeline, along with the gas dynamics, causes variability in composition at compressor stations, where the gas flowing through the pipeline is siphoned to run compressor station engines. Typically, natural gas is composed of a majority methane (CH_4), a small part ethane (C_2H_6), a portion propane (C_3H_8), and the rest by heavier hydrocarbons and inert gasses. However, as noted by the 2014 study of natural gas composition by the Southwest Research Institute [2], the chemical composition in the well alone, dependent on factors such as the organic make up of kerogen which helps produce the natural gas, can vary in Higher Heating Value (HHV) by several hundred btu/scf. The fuel with variability in HHV, as well as other fuel mixture properties, is then fed into an engine along the pipeline which may receive infrequent maintenance, due to inaccessibility, which runs off steady state performance parameters. Concurrently, these parameters set in the engine are tuned to a manufacturer determined optimal level, based upon a tested performance cycle for an expected composition of natural gas. This predetermined optimal level is generally set to reduce the possible damage to the engine when the energy content in the fuel is at a maximum expected level. However, the planning for an outlier case can lead to further issues with reduced engine power and higher Nitrous Oxides (NOx) emission levels when operating off the various sources natural gas fuel running through the engine.

Presently, controllers used to operate these engines account for a small amount of variability, but the engine's themselves can experience problems such as engine damage, auto-ignition, and misfiring if the fuel composition changes drastically. Furthermore, with hundreds of species and thousands of possible reactions occurring with the possible combinations of fuel passing into the engine, the emissions level and power may quickly change as the fuel composition changes. Luckily, GT-Power is a simulation software that can be utilized to obtain combustion characteristics and 'virtual' testing of a controller design before hardware implementation takes place. This process allows for the designed controller to be tested in a virtual environment for fine tuning of the controller to reduce calibration time to the engine and reduce the likelihood of damage occurring to the engine running off new software. The controller designed is to reduce the varied levels of NOx by 50% of current base calibration emissions that results from a varying fuel chemical composition.

CHAPTER II

VARIABLE GAS COMPOSITION

Predictive Indices

When considering the various stable states of the natural gas being extracted during the fracking process, the gas composition can vary widely around an expected state. To account for this, it is generally accepted to use an index to identify the combustible potential of a specific mix to reduce the chance of auto-ignition during the combustion process. [1] One such index, proposed by Leiker at AVL [3], is the Methane Number (MN) to predict auto-ignition within a mixture. MN is defined as the below [3]

$$MN = \left(1 - \frac{Vol_{H_2}}{Vol_{H_2} + Vol_{CH_4}}\right) \times 100 \tag{2.1}$$

The MN number provides an indication of a mix's resistance to auto-ignition, where a low value of the MN will predict a need to retard the ignition timing, to move the ignition timing later in the combustion cycle, to reduce the chance of auto-ignition [1]. This number can thus provide a gauge for the control process to adjust the timing in one direction to correct for the oncoming gas. It is noted that with the presence of diluents, such as CO_2, a MN of over 100 is possible [4]. This index reaching over a value of 100 indicates an auto-ignition tendency below that of even pure CH_4. It is noted in Hedrick et. al [1] that an additional index option is the Wobbe Index (WI) defined as

$$WI = \frac{LHV}{\sqrt{SG}} \tag{2.2}$$

where SG is the specific gravity and LHV is the lower heating value. However, as noted by Hedrick et al [1], a single Wobbe index value can explain multiple different stable states of gas that may be passing through a relay station. Thus, the Wobbe index is not favorable for any ignition controlling criteria since this inaccuracy could result in an over-correction in the ignition timing and cause unnecessary damage to the system.

However, monitoring the MN number is only a single feature to optimize the system around when dealing with a changing gas composition. Additional to this index, as suggested by Hedrick et al [1], the engine performance parameters, such as the laminar flame speed and adiabatic flame temperature, can also be analyzed for optimization. Both of these parameters indicate the instantaneous pressures and temperatures moving through the combustion process, where a deviation from an expected pressure level or temperature level can indicate an increased production in NOx or decrease in engine efficiency. Over time, the peak temperature recorded for differing levels of the air/fuel ratio can provide a graph of the adiabatic flame temperature, as shown below in Figure 2.1.

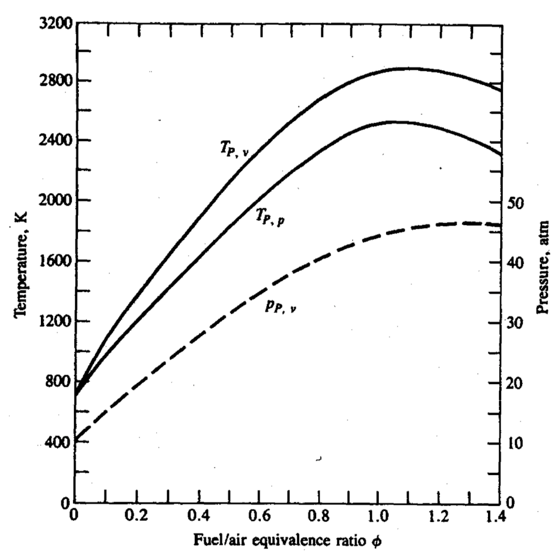

Figure 2.1. Example adiabatic flame temperature curve, taken directly from Heywood [5], pg. 94.

The adiabatic flame temperature curve is compiled from maximum temperature values in a combustion cycle over a range of equivalence ratios. The adiabatic flame temperature is important to note due to the correlation between the level of incomplete combustion products and the temperature of the reaction. For example, the leaner that an engine is running, meaning the lower amount of fuel to air being fed into the engine, will result in less unburned fuel in the exhaust after combustion in the engine's cylinder. Alternatively, the richer the engine is running, the more amount of unburned fuel can pass through the engine at the same operating conditions due to a lower oxygen level not allowing for as complete of a combustion reaction [5]. However, when the engine operates at a higher temperature level, at a higher point on the adiabatic flame temperature curve, the mixture approaches the auto-ignition temperature of the mixture. This situation creates an environment where a spark will create a faster moving flame kernel, correlating to a faster laminar flame speed, allowing for more fuel to be burned during the engines power stroke and resulting in a lowered amount of unburned fuel in the exhaust stroke. While this is advantageous, it is kept in mind that the NOx is exponentially correlated to combustion temperature [6]; however, this can be mitigated by the control system.

Combustion Modeling

While the products of the physical combustion can be evaluated by the use of the above predictive indices, the actual combustion characteristics can also be estimated by the use of computer simulation as well. Currently, the use of CANTERA chemistry solutions can be utilized to develop predictions about the laminar flame speed. This parameter serves to further detail an optimal ignition timing by providing information relative to the combustion reaction speed and reaction timing after spark initiation.

Within CANTERA, a solution can be generated utilizing the GRI-MECH 3.0 solution mechanism, which is a commonly used skeleton for predictions of natural gas combustion. This simulation skeleton encompasses 53 different species of gasses with 325 different reactions [7]. Following predictive species, this simulation environment can yield the laminar flame speed characteristics based upon a one-dimensional laminar flame and follows a multi-component species transport model, code shown in Appendix A given as a demo with the download of CANTERA [7]. The outputs of this code will yield an iterative algorithm resulting in a value for multicomponent flame speed.

CHAPTER III

CONTROLLERS

Controller Scheme

When analyzing the gasses, a NOx sensor will determine the composition of the natural gas flowing through the pipeline. The considered sensors include the NOx 5210 system from ECM, Varian CP -4900 microgas chromatograph, and the GasPT2 from CUI Inc. The benefit of the NOx 5210 system is that it allows two output signals to be broadcasted at once, while at the detriment of accuracy of gas quality measurement. While the NOx 5210 sensor does in fact provide optimal data for combustion exhaust properties, it cannot provide adequate fuel composition data for an intake sensor. Therefore, the comparison between the gas chromatograph and the GasPT2 sensor can be summarized from the PRCI project [8].

The benefit of the gas chromatograph includes the utilization of the thermal conductivity sensor, where a measurement was taken every 3 minutes, and compares the gas composition against a calibrated normal. This thermal conductivity sensor provides data towards the heating properties of the gas travelling past the sensor, providing an accurate measurement relating to the combustion process. This sensor can be calibrated using a certified gas with an expected composition to account for an optimal case passing through the pipeline, where the sensor thus provides a reading deriving from an accurate base case. Alternatively, the GasPT2 sensor is considered an energy sensor; this sensor has a faster response time than the gas chromatograph. There are 2 components to the GasPT2- the main unit is a CO_2 sensor with temperature and pressure sensors, while the secondary unit contains a thermal conductivity sensor and a speed of sound sensor. This sensor provides more data for the combustion properties of the fuel, yielding an optimal option for the system.

For engine controllers, the system is generally represented as a closed loop system. An example closed loop system is represented below in Figure 3.1.

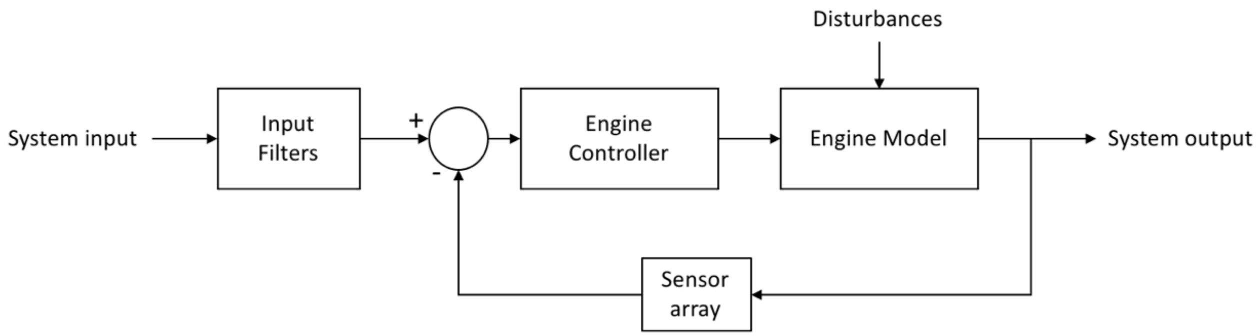

Figure 3.1 Closed loop engine controller. Simplified from [9].

Here, the system inputs include the fuel composition and the engine's initial performance settings. These system inputs will act as the input into the control loop of the control system. As the engine is operated, the engine, and the corresponding model, will encounter external disturbances such as the changing of external humidity, temperature, pressure, and fuel composition. While the engine runs, the output will pass by a sensor array, offering data for the engine controller to adjust based upon operating conditions.

This engine controller, based on the NOx sensor and GasPT2 sensor suggested previously, features a predictive feedback performance where prediction can be determined in the inlet and adjusted based upon the NOx 5210 sensor in the outlet. The data being fed into the engine will thus be generating two data sets for the system to parse. The inlet sensor will provide information relative to an expected combustion curve, following the analysis of the MN and the methane level. Following combustion, the NOx 5210 sensor will provide information relative to the NOx levels emitted in the exhaust. As the noted information is fed to the controller, the data must be passed through a proportional integral derivative (PID) controller to optimize the NOx level during operation. This controller is derived below, from Visioli et al [10], (3.1-3.3) with derivative time constant, τ_D, and integral time constant, τ_1,

$$y(t) = K_c \left(u(t) + \tau_1 \int_0^t u(v)dv + \tau_D \frac{d}{dt} u(t) \right) \tag{3.1}$$

with the transfer function in the ideal non-interacting form

$$transfer(s) = \frac{y(s)}{u(s)} = K_c \left(1 + \frac{1}{\tau_1 s} + \tau_D s \right) \tag{3.2}$$

and further noted in the non-ideal interacting form

$$controller(s) = K_c \left(\frac{\tau_1 s + 1}{\tau_1 s} \right) (\tau_D s + 1) \tag{3.3}$$

where the transfer function (*controller*) is simplified in Skogestad et al [11] (3.4).

$$controller(s) = \frac{K_c}{\tau_1 s} (\tau_1 \tau_D s^2 + (\tau_1 + \tau_D) s + 1) \tag{3.4}$$

This controller features the controller gain, K_c, the integral time, τ_1, the derivative time, τ_D, all represented in the Laplace domain, with notation s. The controller serves to multiply into the differential equation y(s) for the input u(s) to be adjusted towards the target level- In this evaluation equation, y(s) is the NOx level, u(s) is the ignition timing, and $y_s(s)$ are the system inputs described below from Skogestad et al [11].

$$u(s) = K_c \left(\frac{\tau_1 s + 1}{\tau_1 s} \right) \left(y_s(s) - \frac{\tau_D s + 1}{\tau_F s + 1} y(s) \right) \tag{3.5}$$

It is noted that the value of $\tau_F = \alpha \tau_D$ and $\alpha = 0.01$[11]. Skogestad decided to choose the α value as 0.01 to not bias results. This system transfer function, utilized in the above equation form, will thus be utilized by the Simulink model described by the further Model Predictive Control section.

Ignition Timing for Emission Control

The ignition timing is chosen to control the system due to the significant impact on NOx levels. Advancing the ignition timing in the engine cycle allows for the combustion of the fuel to begin further in front of top dead center (TDC) of the piston; TDC of the piston is the location in the combustion process where the trapped volume of the cylinder is minimum [6]. An earlier combustion causes a larger buildup of pressure when the piston reaches TDC since the combustion energy is further increasing the pressure in the cylinder than compression of the gas alone. It is noted that retarding the ignition timing will decrease in-cylinder pressure since the combustion energy will not couple with the compression of the gas, since more fuel will be burned after TDC [6], the later combustion starts in the engine cycle. The larger build up in cylinder pressure from advancing the ignition timing results in a higher in-cylinder temperature increasing NOx formation rates.

GT-Power

GT-Power is a 1-dimensional simulation software where specific components within an engine can be represented as objects with defined mass flow parameters, pressure drops, and expected temperature performances. This software inside Gamma Technologies GT-SUITE allows for the gas dynamics expected through an engine's operation to further predict engine performance. As mentioned before, CANTERA could provide suitable combustion data for a fuel passing through a natural gas engine, providing the necessary information to continue combustion modeling within GT-POWER. This laminar flame speed information, as well as predicted NOx values from the simulation then can be stored for further use by a controller plant.

Model Predictive Control and Simulink

The ultimate system-wide control option would be the Model Predictive Control (MPC) simulation environment to tie the aforementioned control parameters and methods together. The MPC co-simulates an operating environment in multiple areas to generate possible alternatives when organizing the plant of the controller. The MPC model is summarized below, following the design workflow of Chen et al [12], even though the system mentioned is applied to a diesel engine since the controller scheme can be easily applied to natural gas applications.

The MPC system operates off the joint work between the GT-POWER engine model and a Simulink controller. It is important to note that the GT-POWER model and Simulink model are running similar algorithms, but the Simulink model is running the controller code mentioned in the PID section and the GT-POWER model is running combustion simulation based upon the engine components and the CANTERA results. The Simulink model can be represented similarly to Figure 3.1, where the closed loop controller will be adjusting the ignition timing of the physical engine based upon the error introduced by the comparison to the target value from the measured values in the sensor array. The interaction of Simulink and GT-POWER is facilitated by the Simulink interface provided by GT-POWER, which can both drive and collect the necessary measurements from the plant.[12] This interaction follows a verifiable path that the MPC can follow to optimize the performance of the engine, where a simplification is directed by the simulation values. The workflow of the MPC is displayed below in Figure 3.2 reformatted from Chen et al [12].

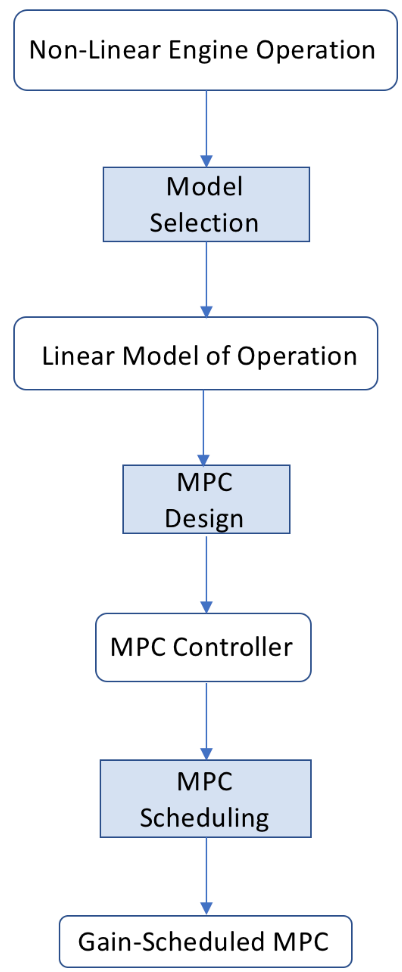

Figure 3.2 MPC controller workflow, reformatted from Chen et al [12].

Naturally, the engine operating in real time, before the onset of the MPC, will be running non-linearly. However, by periodic sampling within Simulink, the engine can be co-simulated between the Simulink measurements and the GT-POWER model. This co-simulation will result in values for maximum temperature/pressure to be compared between the Simulink values and the predicted GT-POWER values. From this co-simulation, a plant function can be selected using tools from the 'System Identification Toolbox' within Simulink. This linearizing plant function will then result in the selection of the appropriate MPC controller, which can be validated by the comparison of the controller performance with predetermined gas compositions; these gas compositions are the expected compositions mentioned previously that could be used to calibrate the sensors. Once this controller is validated based upon a percentage fit between measured values and model values, the controller will be ‘scheduled’ for operation. This scheduling procedure is utilized as a controller selection method in which various ranges of gas compositions will serve as expected operating points; the MPC must be tested and verified at each operating point prior to operation. When the controller is to be scheduled during operation, the system must identify the current operating conditions in respect to the developed schedule, the level of gas compositions, then a finalized gain is utilized for optimum performance until a new gas composition change is detected.

CHAPTER IV

CONCLUSIONS

Analyzing an engine's performance, the changing of the natural gas engine's fuel results in negative effects on the engine's rating, NOx emission levels, and engine efficiency. However, the use of a PID controller to optimize engine performance can be utilized to mitigate these inefficiencies even with a changing fuel composition. Since the PID controller can account for a dynamic changing fuel composition, the negative feedback loop of the controller can adjust the engine's spark timing to continually monitor the reduction in NOx. The controller mentioned can utilize a GasPT2 sensor for upstream gas analysis for chemical composition and a NOx 5210 sensor for the monitoring of NOx emissions. While the GasPT2 sensor monitors CO_2 levels, thermal conductivity, and the speed of sound, expected compositions of fuel traveling through the pipeline can calibrate the sensor to predict the various species in the fuel before reaching the engine by monitoring the MN and the NOx emission levels at constant operating conditions. This calibration can be utilized to prematurely adjust engine parameters in preparation for the changing fuel composition before reaching the engine intake. Thus, the described MPC can collect the necessary information relative to the CANTERA variable fuel combustion estimations, the GT-POWER engine simulation, and the instantaneous Simulink sensor information to provide an optimized controller to minimize the NOx emissions level. Further work moving towards a system of controllers in co-dependence can offer further optimization of two-stroke natural gas engine's models for the optimization of the emission and performance metrics in this industry.

REFERENCES

[1] Hedrick, J., and Jacobs, T. Variable Natural Gas Composition Effects in Lean Burn Two-Stroke Compressor Engines Phase I — Engine Response Final Report. Pipeline Research Council International, 2015. PR-457-14201-R02

[2] Bowles, Ed. "Effect Of Shale Plays On U.S. Natural Gas Composition." Pipeline and Gas Journal, vol. 241, no. 7, July 2014, pgjonline.com/2014/07/14/effect-of-shale-plays-on-u-s-natural-gas-composition/.

[3] M. Leiker et al. "Evaluation of antiknocking property of gaseous fuels by means of methane number and its practical application to gas engines". In: ASME Pap 72-DGP-4 (1972).

[4] S. R. King. "The impact of natural gas composition on fuel metering and engine operational characteristics". In: SAE Technical Papers (1992). doi: 10.4271/920593.

[5] Heywood, John B. Internal Combustion Engine Fundamentals. John B. Heywood. New York : McGraw-Hill, [1988], 1988. isbn: 978-0070286375.

[6] "AP 42, Fifth Edition, Volume I Chapter 3: Stationary Internal Combustion Sources." United States Environmental Protection Agency, US Government, Apr. 2000, www3.epa.gov/ttnchie1/ap42/ch03/index.html. Accessed on 01/20/2018.

[7] C. Developers, Cantera: Chemical kinetics, therodynamics, transport processes, http://cantera.github.com/docs/sphinx/html/index.html, 2012.

[8] Ladd, J., Nuener , B., and Olsen, D. Variable Fuel Composition Air Fuel Ratio Control of Lean Burn Engines. Pipeline Research Council International, 2016. PR-179-13207-R02

[9] Bourn, Gary D., Jess W. Gingrich, and Jack A. Smith. *Advanced Compressor Engine Controls to Enhance Operation, Reliability and Integrity*. Southwest Research Institute (US), 2004.

[10] Visioli A., Zhong QC. (2011) PID Control. In: Control of Integral Processes with Dead Time. Advances in Industrial Control. Springer, London. ISBN: 978-0-85729-070-0

[11] Skogestad, Sigurd. "Simple analytic rules for model reduction and PID controller tuning." *Journal of process control* 13.4 (2003): 291-309.

[12]Chen, R., Maloney, P., Model Predictive Control of Diesel Engine Airpath, Mathworks, 26 Jun. 2013. Webinar.

[13] Hedrick, J. and Jacobs, T. A Review of Variable Natural Gas Composition, Effects, and Control Methods for Reliable Combustion in Lean Burn Two-Stroke Engines. Pipeline Research Council International, 2015. PR-457-14201-R01

[14] Jacobs, T., and Henry H. Predictive Combustion Modeling of Lambertville Large Bore Two Stroke Natural Gas Engine Experiencing Variable Fuel Composition Events. Pipeline Research Council International, 2015.

APPENDIX

Example Cantera Code

```
"""
A burner-stabilized, premixed methane/air flat flame with multicomponent
transport properties and a specified temperature profile.
"""

import cantera as ct
import numpy as np

################################################################
# parameter values
p = ct.one_atm  # pressure
tburner = 373.7  # burner temperature
mdot = 0.04  # kg/m^2/s
comp = 'CH4:0.65, O2:1, N2:3.76'  # premixed gas composition

# The solution domain is chosen to be 1 cm
width = 0.01 # m

loglevel = 1  # amount of diagnostic output (0 to 5)
refine_grid = True  # 'True' to enable refinement

################ create the gas object ########################
#
# This object will be used to evaluate all thermodynamic, kinetic, and
# transport properties. It is created with two transport managers, to enable
# switching from mixture-averaged to multicomponent transport on the last
# solution.
gas = ct.Solution('gri30.xml', 'gri30_mix')

# set its state to that of the unburned gas at the burner
gas.TPX = tburner, p, comp

# create the BurnerFlame object.
f = ct.BurnerFlame(gas=gas, width=width)

# set the mass flow rate at the burner
f.burner.mdot = mdot
```

```
# read temperature vs. position data from a file.
# The file is assumed to have one z, T pair per line, separated by a comma.
zloc, tvalues = np.genfromtxt('tdata.dat', delimiter=',', comments='#').T
zloc /= max(zloc)

# set the temperature profile to the values read in
f.flame.set_fixed_temp_profile(zloc, tvalues)

# show the initial estimate for the solution
f.show_solution()

# don't solve the energy equation
f.energy_enabled = False

# first solve the flame with mixture-averaged transport properties
f.transport_model = 'Mix'
f.set_refine_criteria(ratio=3.0, slope=0.3, curve=1)

f.solve(loglevel, refine_grid)
f.save('ch4_flame_fixed_T.xml','mixav',
    'solution with mixture-averaged transport')

print('\n\n switching to multicomponent transport...\n\n')
f.transport_model = 'Multi'

f.set_refine_criteria(ratio=3.0, slope=0.1, curve=0.2)
f.solve(loglevel, refine_grid)
f.save('ch4_flame_fixed_T.xml','multi',
    'solution with  multicomponent transport')

# write the velocity, temperature, density, and mole fractions to a CSV file
f.write_csv('flame_fixed_T.csv', quiet=False)
f.show_stats()
```