# MINIMAL EMISSION TRAJECTORIES FOR A SUPERSONIC VEHICLE ASCENT PATH 

Mel Human<br>Dept. of Mechanical Engineering<br>North Carolina A\&T State University<br>Greensboro, NC


#### Abstract

In this study, a nitrogen oxide kinetics model is coupled with point mass dynamics and simplified turbojet thermodynamics to form a mathematical model for minimizing NOx formation over a nominal ascent path. The model is one in the variational calculus format which is iteratively solved as a two point boundary problem. Results are given as functions of the equivalence ratio which shows the sensitivity to the fuel throttle setting.


## 1 Background

Aeronautical vehicle emission performance is a critical issue for future generation aircraft as global warming and environmental concerns continue to play important roles in the industry's planning. As air traffic continues to increase at the present rapid rate, it will become increasingly important to exploit all available technologies in order to me the demand, including new propulsion concepts which may not be the most "air friendly" designs. It would be useful to know just how clean a supersonic aircraft may perform with regard to the surrounding environment. Knowing the "best" emission performance would present a basis for evaluating such designs; it's quite possible that the optimal performance may not be adequate for some future environmental requirements.

The production of undesirable combustion products depend on a myriad of factors, including the specific engine design, fuel used, operating conditions, etc. The pollutant of interest will also depend on these factors, for example nitrogen oxides ( NOx ) the subject of this paper are predominant at high combustion
temperatures which encourage the combination of the nitrogen and oxygen molecules. There are numerous kinetic models which simulate the formation of selected species [1-5]. The coupling of an aircraft's flight dynamics with the appro-priests kinetics simulation is the methodology used in this paper.

As the kinetics representation will involve combustion pressures and temperatures, a model must relate system thermodynamics with the thrust dynamics and kinetics. We are concerned with having a flight trajectory which minimizes the overall pollutant formation throughout the entire ascent trajectory, the integral of $N O x$ creation over time will serve as the performance index.

## 2 Pollution Kinetics Model

Depending on the species of interest, there are a number of numerical predictors for substance formation. For this study where we are concerned with nitrogen oxide, we use a model offered by Ritz and Mongia [6]. For complete details refer to the reference, but the key relationships are summarized below:

$$
\begin{align*}
& \text { NOx }\left(\frac{\text { grams }}{\text { kg air }}\right)=  \tag{1}\\
& 0.7 E-16 N_{1} N_{2} T^{1 / 3} \exp \left(0.943 T^{.45}\right)(\tau / 2)^{\alpha}
\end{align*}
$$

where the reaction temperature is
$T=T_{e q} \exp \left(-n\left[1 / \tau^{.7}-1 / \tau_{e q}^{.7}\right]\right)$
the residence time is $\tau$ - taken to be $\mathrm{L}_{\mathrm{cc}} / \mathrm{u}$, and all other parameters are defined in terms of the
equivalence ratio $\phi$. For illustrative puposes we show in Figures 1 show the behavior of two of the model parameters as functions of $\phi$. The model includes additional quantities which also depend on the inlet temperature and pressure such as the a exponent above

$$
\begin{equation*}
n=N 3(\phi)\left(T_{0} / 1090\right)^{N 4(\phi)}\left(P_{0} / 207\right)^{N A(\varphi)} \tag{3}
\end{equation*}
$$

## 3 Vehicle Model

### 3.1 Dynamics

A simplified dynamics formulation is used in the model, a point mass representation with drag and lift characteristics. To assist in the numerical convergence, Cd and Cl values are taken as constant although realistic functions of speed, angle and altitude could be inserted. The two direction second order equations obtained from $F=M a$, are written as a system of four first order equations:
$x^{\prime}=u$
$y^{\prime}=v$
$u^{\prime}=\frac{\tau-\rho A d C d V^{\wedge} 2 / 2}{m} \cos (\alpha)$
$v^{\prime}=\frac{\tau-\rho A d C d V^{\wedge} 2 / 2}{m} \sin (\alpha)+\frac{\rho A l C l V^{\wedge} 2 / 2}{m}$
We will also include a fifth equation which establishes the instantaneous vehicle mass

$$
\begin{equation*}
m^{\prime}=-f m_{a} \tag{4e}
\end{equation*}
$$

where f is the fuel air ratio which may be constant or path position dependent. Not only are these equations subject to initial conditions

$$
\begin{aligned}
& x(0)=0 \\
& y(0)=0 \\
& u(0)=0 \\
& v(0)=0 \\
& m(0)=M_{i}
\end{aligned}
$$

but also four final time requirements (we do not care about the exact final time mass)

$$
\begin{aligned}
& x\left(t_{f}\right)=R \\
& y\left(t_{f}\right)=H \\
& u\left(t_{f}\right)=U \\
& v\left(t_{f}\right)=0
\end{aligned}
$$

Note that we specify the cruise conditions, altitude and velocity at the final time.

### 3.2 Thrust Calculation

The thrust equation is written as

$$
\begin{equation*}
\tau=m_{a}\left[(1+f) u_{e}-u\right] \tag{5}
\end{equation*}
$$

where the mass flow rate is $m_{a}=\rho u A_{i n}$, The density is a function of altitude: $\rho_{0} \exp (-\alpha y)$. Refinements in the mass entrainment such as spillover corrections could be made. The engine's exhaust velocity is [7]

$$
\begin{equation*}
u_{e}=\sqrt{2 C_{p} \eta_{n} T_{c c}\left(1-T_{4} / T_{c c}\right)} \tag{6}
\end{equation*}
$$

where we have compression, heat addition and expansion energy balances

$$
\begin{align*}
& T_{2}=T_{1}(y)\left[\left(p r^{k}-1\right) / \eta_{c}+1\right]  \tag{7a-c}\\
& T_{3}=T_{2}+f \frac{H_{v}}{C_{p}}=T_{c c} \\
& T_{4} / T_{3}=\left[1-\eta_{t}\left(1-p r^{-k}\right)\right]
\end{align*}
$$

Here we account for the variation in the ambient conditions with $T_{\infty}=T_{0} \exp \left(-\alpha_{1} y\right)$ and $p_{\infty}=p_{0} \exp \left(-\alpha_{2} y\right)$.

## 4 Objective Function

Equation which represents the specific NOx creation is the quantity integrated throughout the ascent trajectory is the which we desire to minimize.. The actual integral is

$$
\begin{equation*}
\min \int_{0}^{t_{f}} m_{a} N O x d t \tag{8}
\end{equation*}
$$

Writing out the expression gives

$$
\begin{equation*}
L=\rho u A\left[E(\phi)-F(P, \phi) T^{1 / 3} \exp \left(.943 T^{.45}\right)\right] \tag{9}
\end{equation*}
$$

## 5 The Variational Problem

The model as expressed thus far is in the class of problems referred to as variational calculus optimization or optimal control [8-9]. The integral in Eq. 8 is to be minimized subject to a set of dynamic constraints, Eqs. 4 The driving factor which controls the selected path is some designated control function; in this case, we select the flight angle a as our control variable.

We will merely summarize the solution procedure for such a problem. Denoting the performance index's integrand as L, we construct a optimization objective by adjoining the constraints via a set of Lagrangian multipliers, which actually in this case are called influence functions. Such a result is referred to as the Hamiltonian H

$$
H=L+\sum \lambda_{i} F_{i}
$$

The influence functions are derived from the condition

$$
\begin{equation*}
\lambda^{\prime}=-\frac{\partial H}{\partial x}, \text { or } \lambda_{i}^{\prime}=-\lambda_{i}^{T} \frac{\partial F_{i}}{\partial x} \tag{10}
\end{equation*}
$$

The integration of these functions requires a condition for determining the integration constant, but in this case the conditions are expressed at the final time $t_{f}$. It can be shown that the final time conditions for the multipliers are

$$
\begin{equation*}
\lambda\left(t_{f}\right)=\frac{\partial \phi}{\partial x} \tag{11}
\end{equation*}
$$

which in our case reduces to zero since there is no end point component of the objective function. Note that in the integration process, we must choose initial conditions for the $\lambda$ 's such that final time conditions are satisfied.

In addition, because we are not specifying the final time $t_{f}$ we require an additional condition

$$
\begin{equation*}
\frac{\partial \Phi}{\partial t}+H=0 \quad \text { at } t_{f} \tag{12}
\end{equation*}
$$

Finally the optimal control is determined via the criticality condition

$$
\begin{equation*}
\frac{\partial H}{\partial \alpha}=0 \tag{13}
\end{equation*}
$$

which yields

$$
\begin{equation*}
\tan \alpha=\lambda_{4} / \lambda_{3} \tag{14}
\end{equation*}
$$

## 6 Problem Formulation

### 6.1 General

The theory presented in the previous section can now be applied to our particular problem. We perform one more preliminary step which is the normalization of the variables for the purpose of assisting integration convergence:

$$
\begin{aligned}
& \mathbf{x}=x / R \\
& \mathbf{y}=\mathrm{y} / \mathrm{H} \\
& \mathbf{u}=\mathrm{u} / \mathrm{U} \\
& \mathbf{v}=\mathrm{v} / \mathrm{U} \\
& \mathbf{m}=\mathrm{m} / \mathrm{M}_{\mathrm{i}}
\end{aligned}
$$

(Note that from here on, we are dealing with the normalized quantities). The final problem is presented as:

$$
\begin{aligned}
& \text { minimize } \\
& \int_{0}^{t_{f}} \rho(y) u A\left[E(\phi)-F\left(P_{0}, \phi\right) T^{1 / 3} \exp \left(.943 T^{.45}\right] d t\right.
\end{aligned}
$$

subject to:

$$
\begin{aligned}
& x^{\prime}=u x(0)=0 \quad x(0)=0 \\
& y^{\prime}=v y(0)=0 \quad y(0)=0 \quad y\left(t_{f}\right)=1 \\
& u^{\prime}=c_{1} \frac{u}{m} \exp \left(-\alpha_{1} H y\right)\left(K_{1}-c_{2} u\right) \cos \alpha \\
& u(0)=0 \quad u\left(t_{f}\right)=1 \\
& v^{\prime}=c_{1} \frac{u}{m} \exp \left(-\alpha_{1} H y\right)\left(K_{1}-c_{2} u\right) \sin \alpha \\
& v(0)=0 \quad v\left(t_{f}\right)=0 \\
& m^{\prime}=-c_{3} f u \exp \left(-\alpha_{1} H y\right) \quad m(0)=M_{0} \\
& \lambda_{1}^{\prime}=-\lambda_{3} \\
& \lambda_{2}^{\prime}=-\lambda_{4}
\end{aligned}
$$

$\lambda_{3}{ }^{\prime}=\alpha_{1} \rho_{0} \frac{\partial F 3}{\partial \rho} \lambda_{2}-\lambda_{3} \frac{\partial F 3}{\partial u}-\lambda_{4} \frac{\partial F 3}{\partial v}-\lambda_{5} \frac{\partial F 3}{\partial m}$
$\lambda_{4}{ }^{\prime}=\alpha_{1} \rho_{0} \frac{\partial F 4}{\partial \rho} \lambda_{2}-\lambda_{3} \frac{\partial F 4}{\partial u}-\lambda_{4} \frac{\partial F 4}{\partial v}-\lambda_{5} \frac{\partial F 4}{\partial m}$
$\lambda_{5}{ }^{\prime}=\alpha_{1} \rho_{0} \frac{\partial F 5}{\partial \rho} \lambda_{2}-\lambda_{3} \frac{\partial F 5}{\partial u}-\lambda_{4} \frac{\partial F 5}{\partial v}-\lambda_{5} \frac{\partial F 5}{\partial m}$
$\lambda_{i}\left(t_{f}\right)=0, \quad i=1,2,3,4$
where the derivatives are derived from the right side of equations and

$$
\begin{aligned}
& c_{1}=\rho_{0} A U(1+f) \sqrt{2 C_{p} T_{c c} \eta_{c}} / M_{i} \\
& c_{2}=U / c_{1}(1+f) \\
& c_{3}=\rho_{0} A \\
& K_{1}=\sqrt{1-p r^{-k} \exp \left(-\alpha_{2} H y\right)}
\end{aligned}
$$

### 6.2 Solution Methodology

The described model's solution essentially is based on solving the two point boundary problem defined by the ten differential equations and end conditions. We employed the so called shooting [8] method where initial conditions for the influence functions are iterated upon in order to satisfy the specified final conditions, eight in this case. A set of arbitrary initial conditions are first used to "shoot" to final time values. A vector of errors between the calculated and prescribed end values is computed, and this is used in a Newton Ralplison scheme

$$
J \bullet \Delta X_{0}=-E
$$

where $E$ is the error vector, $J$ is the Jacobian of the system equations, and $\Delta X_{0}$ is the solved for corrections to the initial condition vector.

Because this is a unspecified final time problem, we must utilize the condition Eq. The integration process discussed above is performed for a certain final time until final conditions are satisfied; then Eq. 12 is checked. The process continues until this is achieved.

Throughout the calculation process at each time step the control functions a is derived from $\alpha=\arctan \left(\lambda_{4} / \lambda_{3}\right)$.

## 7 Results and Conclusions

The numerical results are presented in Figures 2 through 5. In Figure 2, we show a plot of the angle control function a as a function of the equivalence ratio $\phi$. For the lower range of $\phi$, there appears to be little difference at different values, in both angle value and functional trend. Toward the upper range, a distinction appears as the vehicle is in a lifting mode during a longer period of time. The corresponding trajectories dictated by this control is shown in the following figure. In both graphs note that the final time is different:

$$
\begin{aligned}
& t_{f}=745,715,695 \text { seconds } \\
& \text { for } \phi=0.3,04,0.6 \text { respectively. }
\end{aligned}
$$

(The slight offset in the graph's endpoint is due to slight errors in scaling the results)

In Figure 4, we show the instantaneous NOx production throughout the three trajectories. The primary reason for the tailing off near the end of the descent is traced to lower temperatures as fuel throttle is lowered. Finally, Figure 5 shows the actual performance index, total ascent NOx production as a function of the equivalence ratio. Higher values clearly escalates the pollution index.

By parameterizing the results in $\phi$, we actually have another control variable f albeit one in which the objective appears monotonic; lower equivalence ratio's yield lower emissions. The actual vlue would depend on other operational factors.

## 8 References

[1] Edelman, R.B., \&Fortune, O.F., "A Quasi-Global Chemical Kinetic Model for the Finite Rate Combustion of Hydrocarbon Fuels with Applications to Turbulent Burning and Mixing in Hypersonic Engines and Nozzles", AIAA paper 69-86, 1969.
[2] Fletcher, R.S., \& Heywood, J.B., "A Model for Nitric Oxide Emissions from Aircraft Gas Turbine Engines," AIAA paper 71-1971.
[3] Hautman, D.J., Dryer, Schug, \& Glassman, "A Multiple-Step Overall Kinetic Mechanism for the Oxidation of Hydrocarbons," Combustion Science and Technology, v. 25, 1981, pp. 603-611.
[4] Rogers, R.C., \& Chinitz, W, "Using a Global Hydrogen-Air Combustion Model in Turbulent Reacting Calculations", AIAA Jour- nal, April, 1983, v.21, \#4, pp. 586-592.
[5] Mongia, H.C., Reynolds, R.S., \& R. Srinivasan, "Multidimensional Gas Turbine Combustion Modeling: Applications \& Limitations," AIAA Journal v. 24, \#6, 1986, pp. 890-904.
[6] Rizk, N.K., \& H.C. Mongia, "NOx Model for Lean Combustion Concept", Journal of Propulsion, Jan. 1995, pp. 161-169.
[7] Hill, P.G., Mechanics and Thermodynamics of Propulsion, Addison Wesley, Reading, Mass., 1965
[8] Bryson, A.E., \& Y. Ho, Applied Optimal Control, Hemisphere Publishing, Wash. D.C., 1975.
[9] Fel'dbaum,A.A., Optimal Control Systems, Academic Press, NT, 1965.

## Nomenclature

E: kinetics parameter
H : cruise altitude - 25kin
$\mathrm{M}_{i}$ : initial vehicle mass $-125,000 \mathrm{~kg}$
Ma: mach number
$\mathrm{N}_{1,2}$ : kinetics parameter
R : range to cruise -75 km
$\mathrm{T}_{\mathrm{cc}}$ : combustion chamber temperature
$\mathrm{T}_{\mathrm{eq}}$ : equilibrium temperature
U : cruise velocity - Mach 2.5
a: kinetics parameter
f: fuel air ratio
u: x velocity
v: y velocity
$\tau$ : thrust
$\alpha$ : vehicle angle
$\phi$ : equivalence ratio
$\Phi$ : final time constraints



