Numerical Prediction of Radiation Measurements Taken in the X2 Facility for Mars and Titan Gas Mixtures

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Thermochemical relaxation behind a normal shock in Mars and Titan gas mixtures is simulated using a CFD solver, DPLR, for a hemisphere of 1 m radius; the thermochemical relaxation along the stagnation streamline is considered equivalent to the flow behind a normal shock. Flow simulations are performed for a Titan gas mixture (98% N$_2$, 2% CH$_4$ by volume) for shock speeds of 5.7 and 7.6 km/s and pressures ranging from 20 to 1000 Pa, and a Mars gas mixture (96% CO$_2$, and 4% N$_2$ by volume) for a shock speed of 8.6 km/s and freestream pressure of 13 Pa. For each case, the temperatures and number densities of chemical species obtained from the CFD flow predictions are used as an input to a line-by-line radiation code, NEQAIR. The NEQAIR code is then used to compute the spatial distribution of volumetric radiance starting from the shock front to the point where thermochemical equilibrium is nominally established. Computations of volumetric spectral radiance assume Boltzmann distributions over radiatively linked electronic states of atoms and molecules. The results of these simulations are compared against experimental data acquired in the X2 facility at the University of Queensland, Australia. The experimental measurements were taken over a spectral range of 310–450 nm where the dominant contributor to radiation is the CN violet band system. In almost all cases, the present approach of computing the spatial variation of post-shock volumetric radiance by applying NEQAIR along a stagnation line computed using a high-fidelity flow solver with good spatial resolution of the relaxation zone is shown to replicate trends in measured relaxation of radiance for both Mars and Titan gas mixtures.

1. Introduction

Spacecraft entering planetary atmospheres at high velocities will experience significant levels of both radiative and convective heating. Depending on the entry velocity and the size of the spacecraft, radiative heating on the vehicle surface could be a significant part of the overall surface heating rate$^1$. Of particular interest to atmospheric entry probe design community are the expected levels of radiative heating for Titan and Mars entries, especially since the current emphasis is on large size entry probes; large sizes are need to accommodate substantially more payload for planetary atmospheric and geological science.

The atmosphere of Titan is composed of primarily diatomic nitrogen (N$_2$) with a small percentage of methane (CH$_4$). The high-temperature shock layer of a vehicle entering the Titan atmosphere will cause the production of cyanogen (CN), which is known to be a strong radiator in the visible region of the spectrum.$^2$ The atmosphere of Mars is composed of primarily carbon dioxide (CO$_2$) and a small percentage of diatomic nitrogen. In addition to CN, the shock layer created during a Martian entry will also contain significant amounts of carbon monoxide (CO) which is a strong radiator in the vacuum ultraviolet (VUV)$^3$. The contributions to radiative heating, and thus overall heating of the atmospheric probe, due to these species must be quantified and validated against flight and/or ground-based experimental data. Since uncertainties are quantified or reduced through the calibration/validation effort, simulation tools can be used with greater confidence in the design cycle.

Computation of radiation from species in the high-temperature shock layer requires precise knowledge of temperatures (kinetic and internal) and number densities of constituent species. Flow environments are typically predicted using modern computational fluid dynamic (CFD) methods. These methods are built around hypothesized models that may include

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thermochemical nonequilibrium effects. Radiation is usually treated as uncoupled from the fluid dynamics. The computed distributions of temperatures and number densities of constituent species from the CFD solution are used as inputs to detailed radiation codes, e.g., NEQAIR and HARA, to determine the distributed surface heating due to shock-layer radiation alone. More recently, attempts have been made to couple the CFD and radiation codes, which can be important if radiation levels are large relative to the overall energy of the flow.

Predictive capabilities are usually calibrated against either ground-based measurements or data gathered from flight. Ground-based facilities that are used to measure spectrally resolved radiation behind a shock front include the NASA Ames Electric Arc Shock Tube (EAST) at NASA Ames Research Center in the US, the Double-Diaphragm Shock Tube (DDST) at the Institute of Mechanics in Moscow, Russia, and the X2 experimental facility at the University of Queensland in Australia. In addition to studying air radiation, experiments have been conducted in recent years in CO₂/N₂ (Mars) and N₂/CH₄ (Titan) gas mixtures. Flight measurements of radiation include FIRE II as well as the more recent Stardust and Hayabusa missions in which attempts have been made to compare results from theoretical computations against airborne observation measurements. Varying degrees of success in simulating experimental measurements numerically indicates that there is still a lot to do both theoretically and experimentally.

An example of a volumetric radiance profile (volumetric spectral radiance integrated over wavelength) seen downstream of a Titan gas mixture shock wave is seen in Figure 1. The radiance upstream of the shock should be negligible due to a (presumably) low freestream temperature. The slight rise in experimental data leading into the shock is probably due to camera artifact known as charge bleed or possibly pre-ionization of the gas. The shock causes a sharp rise in temperature resulting in higher densities and chemical dissociation of the freestream gas into species that are strong radiators, such as CN and CO. Downstream of the shock is a nonequilibrium relaxation zone. The peak temperature and volumetric radiance occur just downstream of the shock (but not necessarily together). The temperatures and species densities in the relaxation zone are in nonequilibrium. The temperatures and volumetric radiance values decrease in the relaxation zone and, depending on the freestream conditions eventually reach equilibrium, or at least steady-state, values further downstream. This portion of the profile will be referred to as the equilibrium plateau.

![Figure 1. Typical experimental volumetric radiance profile in Titan gas mixture (98% N₂, 2% CH₄), shock speed = 5.7 km/s, p=500 Pa.](image_url)

The focus of many previous studies, especially in air, is to match volumetric spectral radiance measurements at the end of the relaxation zone behind a normal shock traveling at a known (measured) shock speed through a chosen gas mixture at a prescribed pressure. The statistical steady state established behind the normal shock is assumed to be the “equilibrium” state – a state that can be predicted using an equilibrium thermodynamic solver such as the CEA code. However, for a relaxing flow, it is not just the end state of relaxation that is important. The path to that final state is equally important. In the
predictive tools, this path depends on the thermodynamic model (single- vs multi-temperature models), chemistry mechanisms, and reaction kinetics (and the dependence of rates on “temperature”). This relaxation is strongly dependent on the freestream pressure (or density), and the strength of the shock in compressing the gas mixture behind the normal shock front – a higher freestream pressure implies quicker relaxation because of increased collision frequency.

The present paper looks at the relaxation process for normal shocks in Mars (CO$_2$/N$_2$) and Titan (N$_2$/CH$_4$) mixtures. Results predicted by the NEQAIR line-by-line radiation code are compared against measurements taken in the University of Queensland X2 Experimental Facility. Previous efforts attempted to employ collision-radiative models to explain any disagreements between theory and experiment. However, in this paper, the flow in the relaxation zone of the X2 shock tube is modeled as a stagnation line of a large blunt body (a hemisphere), with best CFD practices employed to resolve the spatial scale in the relaxation zone.

The primary objective is to determine whether the CFD approach in conjunction with NEQAIR can reproduce the shape of the experimental data in the nonequilibrium relaxation zone. An overview of the X2 facility will be presented as well as a description of the modeling assumptions used by the DPLR CFD code and NEQAIR radiation code. Results will be presented for one Mars gas mixture and six Titan gas mixtures.

II. X2 Facility Overview

A series of experiments aimed at measuring the radiation in air, Mars, and Titan gas mixtures were performed in the University of Queensland’s X2 facility. X2 is a free-piston driven facility that can be operated as either a non-reflected shock tube or as an expansion tunnel and is capable of simulating the shock-layer gas conditions during spacecraft entry into planetary atmospheres at speeds of up to 12 km/s. The facility operates by using a heavy piston to compress and heat a light driver gas until the pressure is sufficiently high (approximately 15.5 MPa) to rupture a 1.2 mm thick pre-scored steel diaphragm. The resulting shock wave is passed through the stagnant test gas in the 85 mm diameter shock tube. The shock leaves the tube into the dump tank as a planar wave and the emission from the heated test gas is analyzed by spectrometers. A schematic of the X2 facility is shown in Fig. 2. Further details of the X2 facility and its capabilities can be found in Refs. 9 and 11.

![Figure 2. Schematic of X2 facility.](image)

Absolute spectral radiance (W/cm$^2$-sr-micron) was measured using an intensified CCD camera coupled to a 300 mm focal length grating spectrometer. Flow behind the shock was imaged onto the entrance slit of the spectrometer giving spatial resolution along the flow axis. The spectrometer was outfitted with a 600 lines/mm grating allowing for the recording of a spectral range of around 140 nm in a single test. The camera was triggered to record with the temporal response of the emission using an exposure time of 100 ns. The spectrometer and camera were calibrated by using a source with a known spectral irradiance. The source was placed in front of the spectrometer and an image was recorded using the same settings as during the tunnel test. Combining this calibrated image with the known magnification of the optical system and losses due to optical surfaces were combined to determine the spectral radiance during the experiment. The spectral radiance was then converted to a volumetric spectral radiance by dividing by the length of the usable core-flow (approximately 60 mm) for each experiment. For this study, numerical results are compared against experimental volumetric radiance and spectral radiance values measured over a spectral range of 310 - 450 nm for both the Mars and Titan gas mixture experiments. In this spectral range, the radiation is primarily due to the CN (violet) band system. A previous study showed that the radiation relaxation rate measured on X2 for Titan gas mixtures agreed very well to the results obtained on EAST.
III. Methodology

A line-by-line radiation code requires temperatures and species number densities along a line-of-sight (LOS). One way to obtain this data is to assume a 1-D normal equilibrium shock, and compute the post-shock state of the gas with an equilibrium code such as CEA. An equilibrium approach, however, will be unable to capture the features of the nonequilibrium relaxation zone shown in Fig. 1. In this paper, the flow quantities downstream of the shock are computed based on a CFD simulation of a 1 m radius hemisphere at the freestream conditions corresponding to the X2 conditions. If there is sufficient angular resolution in the CFD grid around the stagnation line, the bow shock will be normal to the stagnation line of the flow, and hence equivalent to a shock tube simulation. The normal grid lines can be tailored to spatially resolve the nonequilibrium relaxation zone downstream of the shock. The CFD simulations will include the effects of both viscosity and thermal conductivity across the shock. It is intended that by using the best available fluid and thermochemical models in the CFD simulation that accurate inputs will be provided to the radiation code.

Starting from the point where the translational temperature exceeds twice the freestream value, points are selected along the CFD stagnation line solution. The temperatures and number densities at the selected points are duplicated to create a 2-point LOS that is normal to the stagnation line. The length of the LOS is equal to the 60 mm diameter “core-flow” that exits the X2 shock tube. This simulation methodology does not account for any influence of the wall-bounded shear layer.

A. CFD Methodology

The CFD solutions used in this study were generated using v4.02.2 of the DPLR computational fluid dynamic (CFD) code. The DPLR code is a 3-D Navier-Stokes flow solver that has been previously applied to both Mars and Titan entry environments. In this study, DPLR solutions were generated for a hemisphere of 1 m radius, and the stagnation line was taken as representative of the shock tube region of relaxation. A two-dimensional grid of size 160×245 (streamwise × normal) was constructed using GridPro. As the CFD solution progressed, the outer boundary of the CFD grid was tailored to match the shape of the bow shock and to provide adequate spatial resolution of the shock itself.

In addition to chemical nonequilibrium, the flow field was assumed to be in thermal nonequilibrium as well. Consequently, a two-temperature (T-T) model was used. In the two-temperature model employed, the translational and rotational modes of molecules are assumed to be in equilibrium (T=To,rot=To,rot), and are distinct from the vibrational and electronic modes of the molecules; the last two modes are assumed to be in equilibrium (Tv=Tv=To,ele). In a departure from the previous studies for Titan gas mixtures, excited electronic states of the constituent atoms and molecules were included in the present study. For the molecules, CH4, CH2, CH3, HCN, only the ground electronic states, X 1Σ, X 2Σ+, X 1Σ, X 3Π, X 1Σ, respectively, were included, and in doing so, their electronic degeneracies were accounted for in the thermodynamic properties. Inclusion of the excited electronic states does not affect the predicted surface heating but does make a difference in the strength of the radiative signal from the shock front.

For the Titan gas mixture calculations, a 14-species (CH4, CH2, CH3, HCN, N2, C2, H2, CH, NH, CN, N, C, H, and Ar) gas model was used in the computations; the reaction mechanism and rates associated with this model can be found in the work of Gökçen. The Mars computation utilized a 16-species Mars gas model [CO2, CO, CO+, C2, N2, NO, NO+, CN, C, C+, N, O, O+, Ar, e] was used with the Park 1994 reaction rates.

B. Radiation Simulation Methodology

The radiation simulations presented in this paper were produced using the Nonequilibrium Air Radiation (NEQAIR) code. The NEQAIR code is a line-by-line radiation code that computes the radiative emission and absorption along a line-of-sight (LOS) for atomic and molecular electronic and infrared band systems. Individual electronic transitions are evaluated for atomic and molecular species. The code can model the bound-free and free-free continuum radiation caused by interactions of electrons with neutral and ionized atomic species. The external inputs required by NEQAIR are the (nonequilibrium) temperatures and species number densities along a line-of-sight. NEQAIR results have been previously compared against experimental measurements in Mars and Titan gas mixtures taken in the NASA Ames Electric Arc Shock Tube (EAST) facility. Recent improvements to NEQAIR include updating the diatomic Franck-Condon factors for the CN (red and violet), C2 (Swan), and CO (4+) band systems.
For the results presented in this paper, the populations of the excited electronic states are determined using a Boltzmann distribution. Previous studies have shown that the Boltzmann distribution over-predicts radiation for Titan gas mixtures. The NEQAIR code does have a non-Boltzmann (quasi-steady state) model option, but only for air species. The quasi-steady state model in NEQAIR doesn’t extend to the carbon-based species needed for Titan or Mars radiation calculations, so the Boltzmann distribution is used in this study. Because of the overprediction of the Boltzmann results, the absolute values of the NEQAIR and experimental radiation quantities are not compared, but rather, the comparison is limited to the shape of the radiation profiles, thus comparing the rate of radiative relaxation.

The NEQAIR calculations performed in the Mars gas mixture included contributions from the atomic lines of N, O, and C over a spectral range of 310-450 nm. The bound-free and free-continua for O and C were included in the calculation. Diatomic molecular band systems included in the analysis were N2(1+), N2(2+), N2(BH2), NO(β), NO(γ), NO(ε), O2(SR), CN(violet), CN(red), CO(4+), and C2(Swan). The primary contributor to radiation in the spectral range of 310-450 nm is the CN(violet) band system with lesser contributions from the atomic C and O lines. The other band systems are part of the standard NEQAIR Mars model and were retained. As previously stated, the populations of excited energy states were determined using a Boltzmann distribution. Cruden et al. estimated a 30% uncertainty in NEQAIR calculations in Mars gas mixtures. For the Titan calculations, the NEQAIR calculations included contributions from the atomic lines of N, H, and C and the molecular band systems N2(1+), N2(2+), N2(BH2), CN(violet), CN(red), and C2(Swan).

The NEQAIR volumetric radiance profiles are adjusted to take into account the spatial smearing that occurs during the experiment due to the finite time required to gate the cameras. The NEQAIR results are run through a convolution using a unity square function. Essentially, the convolution computes a moving average of the nominal NEQAIR radiance profile over a given spatial interval and smooths out any sharp spikes in the profile. The gate width for all the X2 experiments was 100 ns. For a shock speed of 5.7 km/s, the corresponding smear width would be 0.57 mm. For the cases studied in this paper, the convolution had a noticeable effect only for the 2-3 points immediately behind the shock.

There is a small inconsistency between the flow and radiation simulations. The DPLR CFD solutions were performed under the assumption that the electron temperature, T_e, was equilibrated with the translation temperature. In contrast, the NEQAIR radiation model assumes that the electron temperature is in equilibrium with the vibrational temperature of the gas.

IV. Test Cases

A total of seven X2 test cases were simulated - six with the Titan gas mixture and one with a Mars gas mixture. The uncertainty of the shock velocity was estimated to be ±2.5%. Five of the Titan cases constituted a pressure sweep at a constant shock velocity of 5.7 km/s. The degree of nonequilibrium flow increases with decreasing pressure, but the equilibrium temperature behind the shock increases with increasing temperature. The freestream temperature for all of the cases was assumed to be 300 K.

<table>
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<th>Gas Mixture</th>
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<th>pressure, Pa</th>
<th>temperature, K</th>
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<td>300</td>
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<tr>
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<td>7.6</td>
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</tbody>
</table>
V. Results and Discussion

Experimental data from the Mars and Titan gas mixture X2 tests including volumetric spectral radiance over the wavelength range of 310 - 450 nm and integrated volumetric spectral radiance as a function of distance from the shock. The primary radiator over this spectral range is the CN(violet) band system. In addition, to the volumetric radiance, numerical predictions of temperature and CN number density along the stagnation line will also be investigated.

A. Mars Case

Temperature and CN number density profiles along the stagnation line for the Mars test case are shown in Fig. 3. The peak translational temperature reaches 22000 K at the shock, and thermal equilibration occurs shortly thereafter. The peak CN number density takes place just downstream of the peak temperature location. Because CN radiation intensity is a function of both the temperature and number density of CN, the peak radiance should occur at the shock and decrease as the temperature cool and CN number density decreases along the stagnation line.

![Figure 3. Temperature and CN number density along stagnation line of a hemisphere in Mars gas mixture (96% CO₂, 4% N₂) for a shock speed of 8.6 km/s and pressure of 13 Pa.](image)

The computed and measured volumetric spectral radiance profiles taken at the point of peak radiance downstream of the shock for the X2 Mars test case are shown in Fig. 4a. In order to compare the general shape of the volumetric spectral radiance profiles, the NEQAIR profile has been scaled to match the experimental values at a wavelength of 340 nm. The unscaled NEQAIR peak volumetric spectral radiance was about an order of magnitude larger than the experimental value, a trend similar to that seen in Ref. 12 when Boltzmann distributions were used to model CN radiation in the EAST facility. The shape of the NEQAIR spectrum in Fig. 5a matches the experiment fairly well in the spectral range between 360 and 425 nm, but NEQAIR overpredicts the experiment between 345 and 360 nm.
Figure 4. Comparison of NEQAIR and experimental values, Mars gas mixture (96% CO$_2$, 4%N$_2$) at shock speed of 8.6 km/s and p=13 Pa. Radiation primarily from CN (violet) band system. NEQAIR results are scaled to match experiment at 340 nm and 40 mm. (a) volumetric spectral radiance between 310 and 450 nm. (b) volumetric radiance along stagnation line.

The primary objective of this paper is to determine whether the DPLR-NEQAIR methodology can match the shape of the nonequilibrium relaxation zone downstream of the shock. Figure 4b shows volumetric radiance (volumetric spectral radiance integrated over wavelength) along the stagnation line. The shock location is at x=0 in the figure. To compare the profile shapes, the NEQAIR values were scaled such that they would match the experimental value at x = 40 mm. The peak value of the absolute NEQAIR volumetric radiance was about 3 times larger than the experimental value. The NEQAIR nonequilibrium zone is thinner than that shown in the experimental data, but the shape of the NEQAIR relaxation zone matches the experimental curve very well.

A. Titan Cases

Distributions of temperature and number density (of CN) along the stagnation line of a Titan gas mixture are shown in Fig. 5 for two freestream pressures – 133 Pa and 500 Pa – at a shock speed of 5.7 km/s. The dashed lines in the figures represent the post-shock equilibrium temperature level computed by the CEA code.\textsuperscript{15} In Fig. 5, the red line is translational temperature, the green line is vibrational temperature, and the blue line is CN number density. For the high pressure (500 Pa) case, the approach to equilibrium is quite clear. However, for the low pressure (133 Pa), the gas mixture does not chemically relax to an equilibrium state until the boundary layer edge. The cause for this still being investigated, and it is speculated that the kinetics of one or more exchange reactions in the mechanism needs attention. For either pressure, thermal equilibration is achieved very quickly. In particular, the interaction between the N$_2$ + M $\leftrightarrow$ 2N + M and N$_2$ + C $\leftrightarrow$ CN + N reactions has been shown to control the decay rate for Titan gas mixtures.\textsuperscript{17}
Figure 5. Temperature and CN number density along stagnation line of a hemisphere in Titan gas mixture (98% N\textsubscript{2}, 2% CH\textsubscript{4}) for two different freestream pressures and a shock speed of 5.7 km/s. The dashed line represents the equilibrium post-shock temperature. (a) $p = 133$ Pa. (b) $p = 500$ Pa

Figure 6 shows the volumetric radiance profiles downstream of the shock for 20 and 60 Pa pressure cases at a shock velocity of 5.7 km/s. In all of the Titan results that will be shown, the NEQAIR results are scaled so that the values on the equilibrium plateau (or last data point if there is no obvious plateau) matches the experimental value. The $v=5.7$ km/s, $p=20$ Pa comparison is the best of any of the Titan cases studied. Both the (scaled) peak value and the shape of the relaxation zone predicted by NEQAIR matches the experimental measurements closely. When the freestream pressure is increased to 60 Pa, as seen in Fig. 6b, the shape of the relaxation zone is still matched closely by NEQAIR, but the NEQAIR results show a higher peak value than was measured in X2.

Figure 6. Comparison of NEQAIR and experimental volumetric radiance profiles, Titan gas mixture (98% N\textsubscript{2}, 2% CH\textsubscript{4}) at shock speed of 5.7 km/s. (a) $p=20$ Pa. (b) $p=60$ Pa.

The results for a freestream pressure of 133 Pa and shock velocities of 5.7 and 7.6 km/s are shown in Fig. 7. Similar to the previous figures, the NEQAIR radiance curves have been scaled to match the experimental values on the equilibrium plateau.
As the pressure increases, the spike at the peak volumetric radiance location predicted by NEQAIR becomes larger relative to the experimental data. In addition to the spatial smearing effects due to gate opening, the experimental spike may have been further muted due to effects such as spectrometer resolution. The width of the relaxation zone predicted by NEQAIR is narrower at 7.6 km/s than shown by the experimental data, but in general the shape of the relaxation zone is reasonably well-predicted by the code for the 133 Pa cases.

Results for the two highest pressure Titan cases are shown in Fig. 8. At higher pressures, the width of the relaxation zone is smaller and the extent of the equilibrium plateau is relatively larger than at lower pressures. The peak volumetric radiance values predicted by NEQAIR once again over-predict the experimental values and the width of the relaxation zone computed by NEQAIR at 1000 Pa is smaller than that seen experimentally, but the shape of the relaxation zone predicted by NEQAIR is in close agreement with the experimental profiles.
VI. Conclusions and Future Work

The objective of this paper was to determine if a DPLR CFD solution over a 1 m radius hemisphere using CFD best practices could be used to accurately model the relaxation of volumetric radiance measured in the X2 shock tunnel for Mars and Titan gas mixtures. The X2 experimental measurements were taken over a spectral range of 310-450 nm, where the primary contributor to radiation is the CN(violet) band system. The DPLR solutions accounted for excited electronic states of the constituent atoms and molecules. The stagnation line values from the CFD solution were used to generate the inputs required by NEQAIR. The NEQAIR calculations used the Boltzmann distribution to populate the excited electronic states, an assumption known to over-predict Titan radiation, so the NEQAIR results were scaled to match the experimental data on the equilibrium plateau of the experimental profiles. Generally speaking, the DPLR-NEQAIR solutions matched the experimental shape well for both the Titan and Mars gas mixtures cases, particularly at lower freestream pressure values. Clearly, it would be desirable to match not only the shape of the radiative power density profiles but the absolute values as well. Since the Boltzmann distribution is inadequate (and overly conservative) when modeling CN radiation, a more suitable distribution function should be found. If an effective non-Boltzmann excited states distribution model could be developed for Titan and Mars gas mixtures, the DPLR-NEQAIR methodology has the potential to accurately simulate CN radiation in these flows.

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VIII. References


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27 Rodio, J., [PLACEHOLDER FOR RODIO REFERENCE]