THE PROGRESS IN SIMULATION OF NITROUS OXIDE MONOPROPELLANT OPERATION

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ABSTRACT

The computer model for simulation of nitrous oxide (N_2O) monopropellant thruster operation is presented. In the thruster a flow of N_2O injected into the reaction chamber decomposes on pre-heated catalyst. The products of the decomposition leave the chamber through the nozzle producing thrust. For modelling the thruster is considered an open system divided in six control volumes (CV). The catalyst is modeled as a porous medium; conductive, convective and radiation heat transfer between CV's and ambient are taken into account. The model simulates the thruster's performance during transient and steady-state modes of operation. N_2O monopropellant operation has been simulated and satisfactory match between experimental data and computational results is achieved during model validation. Recent improvements in the computer code include expansion of the number of considered gas mixture species from 3 to 13 and more accurate calculation of gas mixture transport properties.

KEYWORDS: nitrous oxide, N_2O, monopropellant thruster, space propulsion

NOTATIONS

NIST = The National Institute of Standards and Technology
A, A_t = hydraulic cross-sectional areas for chamber and nozzle throat respectively, m^2
A_a, A_c, A_s, A_r, A_{th} = surface areas for external casing, catalyst, internal casing, radiation, and thermal insulation respectively, m^2
a = relative mass N_2O concentration
a_0 = initial relative mass N_2O concentration of injected propellant
C_p, C_c, C_s, C_h, C_{th} = specific heat capacities for gas, catalyst, casing, heater, and thermal insulation respectively, J/kg/K
CV= control volume
D_{N2O} = N_2O diffusion coefficient, m^2/s
E_{am}, E_{at} = activation energies for homogeneous and heterogeneous reactions respectively, kJ/mol
H_0, H = initial and current flow specific enthalpies respectively, J/kg
h_c, h_s, h_{amb} = convective heat transfer coefficients for catalyst, casing, and ambient respectively, W/m^2/K
I_{sp} = specific impulse, s
k_m, k_t = pre-exponential factors for homogeneous and heterogeneous reactions respectively, 1/s
m, m_c, m_s, m_h, m_{th} = gas, catalyst, casing, heater, and thermal insulation masses respectively, kg
$\dot{m}$, $\dot{m}_{in}$, $\dot{m}_{out}$ = propellant mass flow rates through, into, and out of chamber respectively, kg/s
P = heater power, W
p, p_0, p_c, p_{amb} = chamber, stagnation, critical flow, and ambient pressures respectively, Pa
Q = specific heat of reaction, J/kg
R = ideal gas constant, R = 8.314472 J/mol/K
r, r_s, r_h, r_{th} = chamber, casing, heater, and thermal insulation radii respectively, m
S = specific surface area for catalyst, m^2/kg
SLPM = standard litres per minute
T, T_0, T_c, T_s, T_h, T_{th}, T_t, T_{amb} = gas, stagnation, catalyst, casing, heater, thermal insulation, nozzle throat gas flow, and ambient temperatures respectively, K
t = time, s
V = chamber volume, m^3
v, v_s = flow and sonic velocities respectively, m/s

W_m, W_t = reaction velocities for homogeneous, kg/m^3/s, and heterogeneous, kg/m^2/s, decomposition respectively
Nu, Re, Pr, Gr = Nusselt, Reynolds, Prandtl, and Grasgoff numbers respectively
ε = emissivity
μ = molar mass, kg/mol, μ = 44.013 g/mol for N_2O
ρ_0, ρ_t, ρ = gas stagnation, nozzle throat, and mixture densities respectively, kg/m^3
σ = Stephan-Boltzmann constant, $\sigma = 5.67\times10^{-8}$, W/m^2/K^4
γ = specific heats' ratio for a gas
λ = dimensionless flow velocity
λ, λ_c, λ_t, λ_h, λ_{th} = thermal conductivity coefficients for gas, catalyst, material, heater, and thermal insulation respectively, W/m/K
ξ = catalyst porosity
η = viscosity, Pa s
abs. = absolute value

1. INTRODUCTION

Nitrous oxide (N_2O) has been considered a "green" [1] alternative to hydrazine propellant for small satellite propulsion. [1]-[3] N_2O monopropellant thruster prototypes have been built and successfully fired in the U.K. [3], China [4]-[6], Russia [7], and the U.S. [8]. These thrusters employ catalysts for N_2O decomposition. In such a device, shown schematically in Figure 1, a flow of nitrous oxide is injected into the reaction chamber. Upon injection, nitrous oxide decomposes on a pre-heated catalyst. The products of the decomposition leave the chamber through the nozzle producing thrust. Once balance between heat generation by decomposition and heat dissipation into the surrounding environment is achieved the reaction becomes self-sustaining so that heating input is no longer required. Specific impulse performance for the prospective N_2O monopropellant in Figure 2 is a function of decomposition temperature that reaches maximum Isp=206 s at about 1640 ºC. This makes N_2O monopropellant a suitable option for spacecraft station-keeping and small orbit maneuvers.

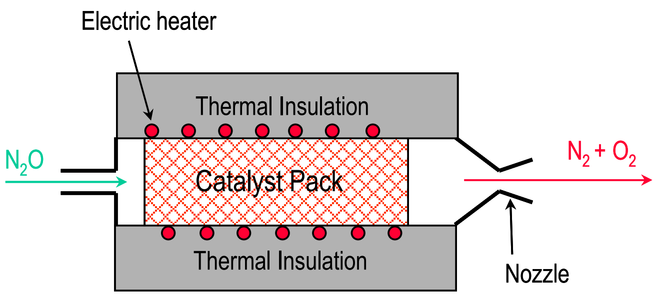

Figure 1. Nitrous oxide monopropellant thruster schematics.

Lack of a tool for simulation of an N_2O monopropellant operation had made engineers rely on their experience in designing these devices before the computer model has been developed for this purpose. The computer model for the simulation of an N_2O monopropellant operation has been validated for the range of pressures and mass flow rates. [9]

In the model presented in reference [9] N_2O decomposition is restricted to a single exothermic reaction: $N_2O \rightarrow N_2 + \frac{1}{2}O_2$. A program block calculating multi-component composition of the reacting gas mixture and its properties has been recently added to enhance the model. This paper describes the computer model and the recent improvements in simulation of multi-component composition of the reacting gas mixture.

[1] propellant with no or negligible toxic or carcinogenic risk

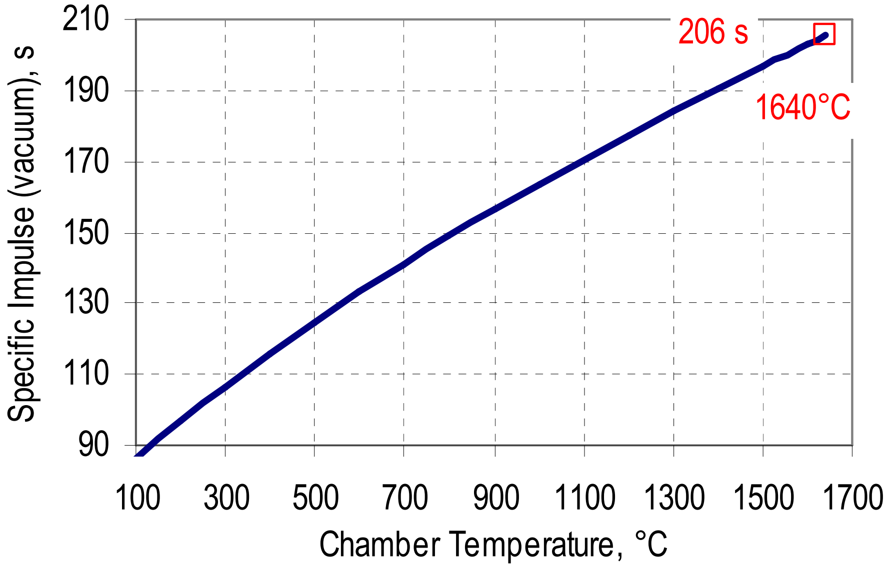

Figure 2. Theoretical specific impulse performance for N_2O monopropellant as a function of chamber temperature. (for nozzle expansion ratio 200)

2. N_2O MONOPROPELLANT DESIGN AND OPERATION

Inside the decomposition chamber of the N_2O monopropellant thruster design shown in Figure 1 pellet catalyst is packed into a cylindrical shape. Electric heater curled around the outer of the chamber's casing warms up the catalyst. Thermal insulation around the heater reduces heat transfer losses into surrounding environment.

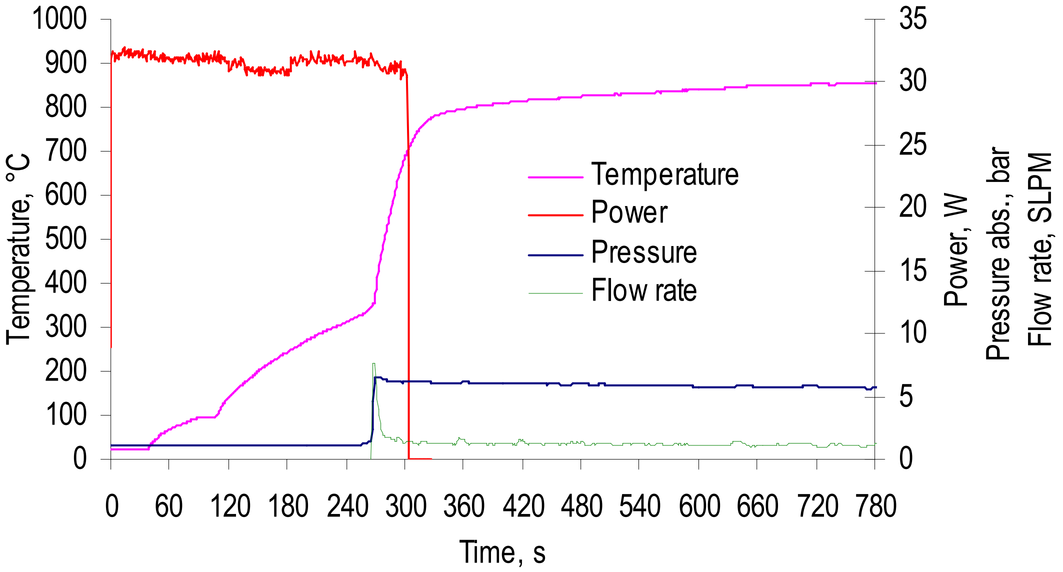

Figure 3. Experimental output readings for test 297.

The acquired readings for a typical N_2O monopropellant thruster prototype firing are shown in Figure 3. During the run electric heater was first turned on for ~4.5 minutes to warm up the catalyst, then the flow of N_2O was on. Since that moment an initiated N_2O decomposition reaction is responsible for steep rise of the temperature inside the thruster. After in-flow thermocouple reading climbed up to ~700ºC electric power was switched off. Lacking the heating power input the temperature of self-sustaining decomposition reaction stabilized at about 850ºC.

3. MODEL

In comparison to the earlier model described in reference [9] in this model the thruster is divided in six control volumes (CV): gas inside chamber, catalyst, casing, heater, thermal insulation, and nozzle shown in Figure 4 instead of five ones. The extra CV has appeared after the heater CV in reference [9] had been split into two CVs: heater and thermal insulation. Although this split increased the model complexity more accurate heater and thermal insulation temperature values have been obtained. The physical properties of each CV are uniform.

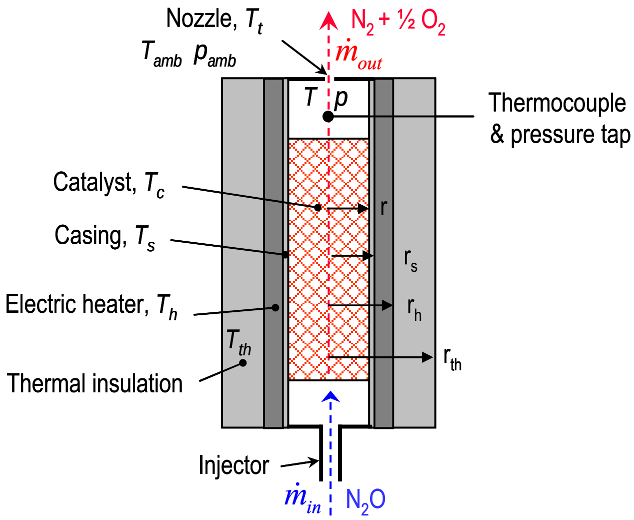

Figure 4. N_2O monopropellant calculation model.

For gas inside the chamber, heat generated by decomposition reaction is spent for the flow heating, and heat transfer with catalyst and casing, so that the heat rate balance is as:

$$\left(VW_m + A_c W_t\right)Q + \dot{m}\left(H_0 - H\right) - h_c A_c \left(T - T_c\right) + h_s A_s \left(T_s - T\right) = 0$$

Equation 1

Nitrous oxide decomposition inside the chamber is assumed to follow the equation: $N_2O \rightarrow N_2 + ½O_2$. This is an exothermic reaction with the standard heat release Q=82 kJ/mol [10].

Inside the thruster, N_2O decomposition occurs not only in-flow (homogeneous) but also on the catalyst surface (heterogeneous).

The reaction velocity for homogeneous decomposition is calculated as [11]:

$$W_m = a\rho k_m e^{-\frac{Eam}{RT}}, \text{ kg/m}^3\text{/s}$$

Specified data for activation energy (E_{am} = 249.434 kJ/mol) and pre-exponential factor (k_m=1.3×10^{11} 1/s) for homogeneous N_2O decomposition reaction have been taken from NIST Chemistry WebBook [12]

Heterogeneous reaction velocity is calculated as [13]:

$$W_t = a\rho\sqrt{D_{N2O} k_t e^{-\frac{Eat}{RT}}}, \text{ kg/m}^2\text{/s}$$

Activation energy (E_{at}) and pre-exponential factor (k_t) are specific for each catalyst and should be found empirically.

The catalyst is considered being a porous medium for which the heating rate is determined by thermal conductivity with the thruster casing and convective heat transfer with gas:

$$C_c m_c \frac{dT_c}{dt} = \frac{2\pi l}{\frac{1}{\lambda_c}\ln\frac{r_c}{r_{gc}} + \frac{1}{\lambda_s}\ln\frac{r_{gs}}{r_c}}\left(T_s - T_c\right) + h_c A_c \left(T - T_c\right)$$

where r_{gc}, r_{gs}, r_{gh} and r_{gth} are bulk heat capacity "gravity" centers for catalyst, casing, heater and thermal insulation respectively calculated on a basis of radii parameters, shown in Figure 4, according to the formulae:

$$r_{gi}=\frac{\int_a^b 2\pi r\rho_i C_i r dr}{\int_a^b 2\pi r\rho_i C_i dr}=\frac{\int_a^b r^2 dr}{\int_a^b r dr}=\frac{2}{3}\frac{b^2+ab+a^2}{a+b}$$

for catalyst: $i\equiv c\Rightarrow$ $a=0$, $b=r_c$
for casing: $i\equiv s\Rightarrow$ $a=r_c$, $b=r_s$
for heater: $i\equiv h\Rightarrow$ $a=r_s$, $b=r_h$
for thermal insulation: $i\equiv th\Rightarrow$ $a=r_h$, $b=r_{th}$

The thermal conductivity of the porous medium is determined from a theoretical value for material as [14]: $\lambda_c=\lambda_t(1-\xi)$, while the catalyst surface area is found from its mass multiplied by the specific surface of the substrate: $A_c=m_c S$.

The heat rate absorbed by the casing CV is equal to the sum of the rates transferred through the CV by conductivity between heater and catalyst, by convection from gas inside the chamber to the ambient, as well as by radiation to the ambient:

$$C_s m_s\frac{dT_s}{dt}=\frac{2\pi l}{\frac{1}{\lambda_s}\ln\frac{r_s}{r_{gs}}+\frac{1}{\lambda_h}\ln\frac{r_{gh}}{r_s}}(T_h-T_s)-\frac{2\pi l}{\frac{1}{\lambda_c}\ln\frac{r_c}{r_{gc}}+\frac{1}{\lambda_s}\ln\frac{r_{gs}}{r_c}}(T_s-T_c)-h_s A_s(T_s-T)$$
$$-h_{amb}A_a(T_s-T_{amb})-\sigma\varepsilon A_r\left(T_s^4-T_{amb}^4\right)$$

The electric power input in the heater CV is converted to heat increasing it's temperature and transferred to the thruster's casing and thermal insulation by thermal conductivity:

$$P=C_h m_h\frac{dT_h}{dt}+\frac{2\pi l}{\frac{1}{\lambda_s}\ln\frac{r_s}{r_{gs}}+\frac{1}{\lambda_h}\ln\frac{r_{gh}}{r_s}}(T_h-T_s)+\frac{2\pi l}{\frac{1}{\lambda_h}\ln\frac{r_h}{r_{gh}}+\frac{1}{\lambda_{th}}\ln\frac{r_{gth}}{r_h}}(T_h-T_{th})$$

Equation 2

The thermal insulation is for reduction of heat losses out of the thruster. Its heating rate is determined by heat transfer from the heater by conductivity and heat removal to the ambient:

$$C_{th}m_{th}\frac{dT_{th}}{dt}=-\frac{2\pi l}{\frac{1}{\lambda_h}\ln\frac{r_h}{r_{gh}}+\frac{1}{\lambda_{th}}\ln\frac{r_{gth}}{r_h}}(T_{th}-T_h)-h_{amb}A_{th}(T_{th}-T_{amb})$$

Convective heat transfer coefficients (h_c, h_s, h_{amb}) are calculated using Nusselt number $Nu=1.18(GrPr)^{0.125}$ for free (no flow) and $Nu=0.41Re^{0.6}Pr^{0.33}$ for forced (flow) convection cases. [14]

The flow of hot reaction products is choked by a cylindrical nozzle at the chamber's exit. Isentropic flow of ideal gas is assumed for the nozzle flow calculation [15]:

$$\frac{T}{T_0}=1-\frac{\gamma-1}{\gamma+1}\lambda^2;\ \frac{\rho}{\rho_0}=\left(\frac{T}{T_0}\right)^{\frac{1}{\gamma-1}};\ \frac{p}{p_0}=\left(\frac{T}{T_0}\right)^{\frac{\gamma}{\gamma-1}}$$

where dimensionless flow velocity (λ) is referred to sonic velocity at nozzle throat (v_s): [15]

$$\lambda=\frac{v}{v_s};\ v_s=\sqrt{\gamma\frac{R}{\mu}T_t}$$

Sonic flow through the nozzle is determined by the following criterion [15]:

$$\frac{p_{amb}}{p_0}\geq\frac{p_c}{p_0}=\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}}$$

Equation 3

Continuity equation, $\frac{dm}{dt} = \dot{m}_{in} - \dot{m}_{out}$, is suitable for both transient and steady state flow cases. Propellant mass flow rate ($\dot{m}_{out}$) is determined by flow through the nozzle. The data for propellant mass change $\frac{dm}{dt}$ inside the chamber are derived from experimental pressure readings, calculated temperature and gas mixture composition, knowing the chamber's volume.

Ideal gas law is used for calculation of concentration and density inside the chamber. Determination of reaction products' composition is necessary for accurate assessments of thermodynamic and transport properties for gaseous mixture. A single exothermic decomposition reaction ($N_2O \rightarrow N_2 + \frac{1}{2}O_2$) was considered in the previous versions of the model. In the current model list of considered species has been extended to: N_2O, N, O, N_2, O_2, N_3, O_3, NO, NO_2, NO_3, N_2O_3, N_2O_4, and N_2O_5. Chemical composition of reaction products is calculated by equilibrium constant method. [16] The necessary thermodynamic data (μ, C_p, γ, H, K_p) have been calculated by the data and procedures from NASA Lewis publications. [17] Transport properties for gaseous mixture (λ, η, D_{N2O}) are calculated using the procedures taken from Lawrence Livermore National Laboratory report. [18] Transport properties for single components and binary mixtures are taken from NASA Lewis publications. [19]

The problem is divided into 2 parts: simulation of N_2O decomposition inside the reaction chamber, and flow of reaction products through the nozzle. Since decomposition reaction rate inside the chamber depends on the N_2O mass flow rate that is restricted by the nozzle, and vice versa, the flow rate through the nozzle relies on conditions inside the chamber determined by the reaction rate, an iterative approach is used for the solution.

3.1. *Algorithm*

The main goal set was to simulate the N_2O monopropellant operation during the most important, start-up transient and steady-state, thruster modes.

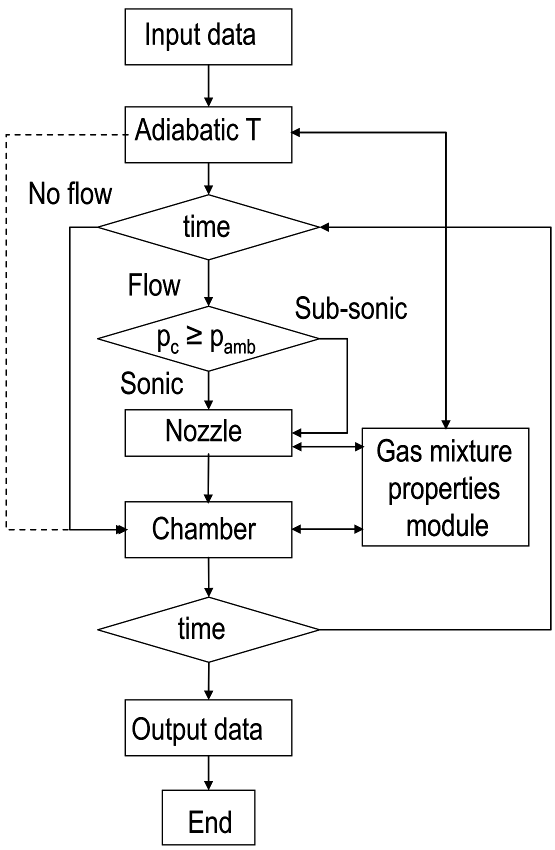

Figure 5. Model algorithm.

The model has been programmed into a FORTRAN code using the computational algorithm given in Figure 5. The program starts with uploading input data including initial temperatures, chamber, catalyst, and nozzle sizes, catalyst, casing, and heater masses as well as their thermal properties. Chamber pressure and heater input power data acquired real-time during the experiment are fed into the program, and are used at each time step for calculation of the rest of the performance. Maximum temperature achieved for the reaction is then determined by equating enthalpies for reactants and products by secant method while assuming adiabatic process for complete N_2O decomposition. This value is later used as an initial maximum temperature guess while ambient temperature is an initial minimum temperature guess for equation 1. The next step is the beginning of a time loop when the choice is made from three possible cases: thruster heating and no flow; heating and flow; no heating and flow.

The first case corresponds to the starting phase of the thruster operation when the catalyst is pre-heated. Since there is no in-flow and no decomposition, the first term in equation 1 associated with chemical reaction vanishes so that the equation changes to: $mC_p \frac{dT}{dt} - h_c A_c (T - T_c) + h_s A_s (T_s - T) = 0$. Because the gas inside the chamber expands on heating there is still a small flow through the nozzle, and the continuity equation changes to: $\frac{dm}{dt} = \dot{m}_{out}$.

The second case is in start-up transient when both heating and flow are on, and the nozzle flow condition (non-choked or choked) is crucial for the decomposition reaction rate. For this case, the condition by equation 3 is applied to find out if the flow in the nozzle is sonic or sub-sonic. For a sub-sonic flow velocity through the nozzle is found by: $\lambda^2 = \frac{\gamma+1}{\gamma-1}\left[1 - \left(\frac{p_{amb}}{p_0}\right)^{\frac{\gamma-1}{\gamma}}\right]$ For sonic flow $\lambda = 1$, so that $\frac{T}{T_0} = \frac{2}{\gamma+1}$. Steady state is achieved promptly after the flow is turned on, and continuity is applied as: $\dot{m}_{in} = \dot{m} = \rho v A = \dot{m}_{out} = \rho_c v_c A_t$ since $\frac{dm}{dt} = 0$.

The third case is when the heater power is off so that left-hand-side of equation 2 vanishes, giving. $0 = C_h m_h \frac{dT_h}{dt} + \frac{2\pi l}{\frac{1}{\lambda_s}\ln\frac{r_s}{r_{gs}} + \frac{1}{\lambda_h}\ln\frac{r_{gh}}{r_s}}(T_h - T_s) + \frac{2\pi l}{\frac{1}{\lambda_h}\ln\frac{r_h}{r_{gh}} + \frac{1}{\lambda_{th}}\ln\frac{r_{gth}}{r_h}}(T_h - T_{th})$

Once the choice is made equation 1 is solved for T by bisection method, and the other temperatures are calculated explicitly. This has been found by experience to be the most suitable method for the case. At the end of the time loop the results are printed as a table for further analysis.

3.2 *Results and Discussion*

The calculation results of the two models have been compared to the experimental ones in Figure 3. The comparison results are illustrated in Figure 6. Since the experimental chamber pressure and heating power data are input read in the algorithm they are not shown in Figure 6.

The results plotted in Figure 6 demonstrate that the flow temperature values predicted by the both models are close to the experimental ones. The r-squared values [2] for gas flow temperature fit between the experiment and calculation are 0.998 for previous and 0.997 for current model. The current model predicts slightly higher propellant mass flow rate then the previous one. For flow rate fit the r-squared values are 0.654 for previous and 0.688 for current model representing better fit between

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[2] r-squared value is a square of the Pearson product moment correlation coefficient: $r = \frac{\sum(x-\bar{x})(y-\bar{y})}{\sqrt{\sum(x-\bar{x})^2 \sum(y-\bar{y})^2}}$. It can be interpreted as the proportion of the variance in y attributable to the variance in x.

the current model and experimental readings. It can, therefore, be concluded that the nitrous oxide decomposition ($N_2O \rightarrow N_2 + ½O_2$) is the dominating reaction for the considered temperature range and the contribution of the other reactions involving N, O, N_3, O_3, NO, NO_2, NO_3, N_2O_3, N_2O_4, N_2O_5 chemical species gives about 3% enhancement of the model accuracy. The next significant improvement is viewed in extending the model to 1-dimensional geometry.

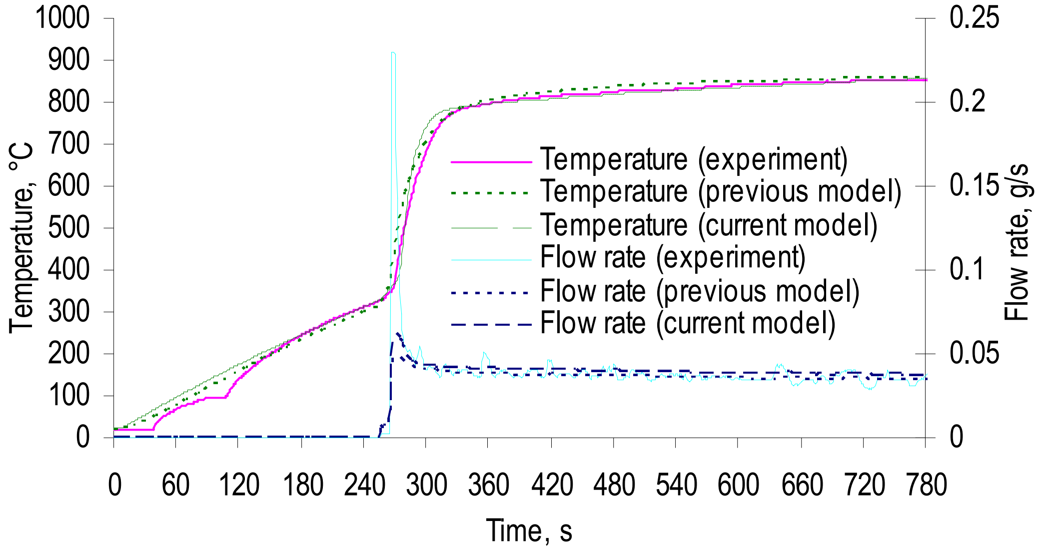

Figure 6. Comparison of experimental and simulation results for test 297.

4. SUMMARY

The model under development is the tool for simulation of nitrous oxide monopropellant thruster operation. The earlier version of the model was validated by comparison to the experimental data. The correlation between the experimental and simulation results represented by r-squared values (r^2=0.998 for temperature and r^2=0.654 for flow) is satisfactory for preliminary assessments of average operation performance and optimization of monopropellant thruster design.

The recent improvements to the model add about 3% accuracy (r^2=0.688) in propellant flow prediction. Further development of the model is suggested to focus on 1-dimensional geometry.

ACKNOWLEDGEMENT

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