Numerical Study of Chemical Performance of 30 ton$_f$-class LRE Nozzle of KARI

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Abstract

Three methods of nozzle flow analysis, frozen-equilibrium, shifting-equilibrium and non-equilibrium approaches, were used to rocket nozzle flow, those were coupled with the methods of computational fluid dynamics code. For a design of high temperature rocket nozzle, chemical equilibrium analysis which shares the same numerical characteristics with frozen flow analysis can be an efficient design tool for predicting maximum thermodynamic performance of the nozzle. Frozen fluid analysis presents the minimum performance of the nozzle because of no consideration for the energy recovery. On the other hand, the case of chemical-equilibrium analysis is able to forecast the maximum performance of the nozzle due to consideration for the energy recovery that is produced for the fast reaction velocity compared with velocity of moving fluid.

In this study, using the chemical equilibrium flow analysis code that is combined the modified frozen-equilibrium and the chemical-equilibrium. In order to understand the thermochemical characteristic components and the accompanying energy recovery, shifting-equilibrium flow analysis was carried out for the 30 ton$_f$ - class KARI liquid rocket engine nozzle together with frozen flow. The performance evaluation based on the 30 ton$_f$ - class KARI LRE nozzle flow analyses will provide an understanding of the thermochemical process in the nozzle and performances of nozzle.

Introduction

It come to thousand of the degree that the temperature of the combustor doing an oxidizer with hydrocarbon series fuel and oxygen like as the KSR-III rocket. The flow of rocket nozzle should undergo change a seriously temperature and pressure variation because of the expansion into a short time to the external atmosphere condition. The chemical formation being a dissociation state after combustion is recombined due to the reduction with temperature at the expansion process, and then an amount of heat using the thermal dissociation is restored. Accordingly, the chemical elementally construction is generated a large difference at the combustor and nozzle exit, and a correct prediction of elementally construction should be calculated the responsible thermochemical performance. A responsible solution should not obtain at the design process of rocket by an analysis with frozen-equilibrium not considering variation of a chemical composition and property of matter as the temperature change.[1]

It is separated the chemical-equilibrium, to consider the chemical last condition, and non-equilibrium analysis, to consider the reaction velocity, by the method with a variation of the chemical construction. The method with the concision of elementally should be used to solve the chemical-equilibrium equations in the each step because equilibrium and non-equilibrium analysis doesn’t remain the existing data in the combustion product of hydrocarbon fuel.

In the frozen-equilibrium analysis, the minimum performance of nozzle is presented because of no consideration with the energy recovery of nozzle, on the other hand, the case of chemical-equilibrium analysis is represented the maximum thermal energy recovery owing to a quick reaction velocity compared with a flow velocity, and it should predict the maximum performance of nozzle. It should be accomplished to the reaction velocity analysis, namely non-equilibrium, with recombination velocity for the correct prediction. However, in proportion as increase the species, the increased equations have a disadvantage with expanding calculation, and it has the issue of efficiency.

The non-equilibrium is became a generalization with a prediction of correct result already, but the equilibrium has a meaning in that should be better a relatively convergence characteristic and represented a maximum limit of nozzle performance.[2]

In this study, it was used that the existing frozen-equilibrium and a revision code, namely the chemical-equilibrium analysis code, with hydrocarbon fuel. In this analysis, there is analyzed a performance of the 30 ton$_f$-class KARI LRE, and this study inquire into a difference of each analysis result and theoretical result.

Numerical Approach

Frozen and equilibrium equations

In this study, the considering equations of frozen and equilibrium express the vector form as following.

$$\frac{\partial Q}{\partial t}+\frac{\partial F}{\partial \xi}+\frac{\partial G}{\partial \eta}+\frac{1}{r}H=0 \quad (1)$$

$$Q=\left(\rho,\ \rho u,\ \rho v,\ e\right)^T \quad (2)$$

Here, in case of a considering variation according to a chemical construction change and specific temperature, the total energy and pressure defines as following.

$$e=\sum_{k=1}^{NS} x_k\left(\int_{T_{ref}}^{T}\frac{C_{c_k}}{M_{w_k}}dT+H_{f_k}^{0}\right)+\frac{\rho}{2}\left(u^2+v^2\right) \quad (3)$$

$$p=\rho RT/\sum_{k=1}^{NS} x_k M_{w_k} \quad (4)$$

The equation should be analyzed by the way of a existing frozen-equilibrium analysis, but the specific heat and pressure obtained a temperature and accomplish the temperature calculation from Eq. (3). Moreover, a part out of the partial derivative of pressure should be modified in existing solution for the accuracy and stability.[3,4] In the Eq. (3,4), the mole fraction x_k obtained from the chemical-equilibrium computing of next paragraph, and the computing temperature and pressure are re-used the equilibrium construction computing and then are formed a repeated computing at Eq. (3,4). In other hand, in independent of a temperature and pressure, the mole fraction x_k become a solution of frozen-equilibrium with the considering specific heat by the function of temperature. It was used NASA Polynomial Fit that temperature and equilibrium constant computing using the thermochemical data.[5]

Chemical-equilibrium analysis

The production of the hydrocarbon fuel is (CO_2, CO, H_2O, OH, O_2, H_2, O, H, N_2) In the chemical reaction analysis, and nitrogen assumed inactivity. In this case, the combustion of any hydrocarbon fuel is represented as following a general reaction.

$$\begin{aligned}C_xH_y+a\left(O_2+3.76N_2\right)\rightarrow\ & x_1CO_2+x_2CO\\ &+x_3H_2O+x_4OH+x_5O_2\\ &+x_6H+x_7O+x_8H+x_9N_2\end{aligned} \quad (5)$$

Here, it is chemical-equilibrium equation with the function of elementally conservation form, temperature and pressure about each element to need the ration of elementally for computing.

$$\begin{aligned}&R_{C/O}=x/2a,\ R_{H/O}=y/2a,\\ &R_{N/O}=3.76,\ \sum_{k=1}^{NS}x_k=1\end{aligned} \quad (6)$$

$$\begin{aligned}&2CO_2\leftrightarrow 2CO+O_2\ ,\ 2H_2O\leftrightarrow 2H_2+O_2\\ &O_2+H_2\leftrightarrow 2OH\ ,\ H_2\leftrightarrow 2H\ .\ O_2\leftrightarrow 2O\end{aligned} \quad (7)$$

The above Eq. (6), (7) is an algebraically simultaneous equations of closed type, and should be solved the Newton iteration.

There is calculated the combustion temperature, pressure and chemical construction for the inlet condition of nozzle flow. Assuming the pressure of combustor in relation to mass flow rate is 60bar, the temperature and chemical construction commutated using the chemical-equilibrium and enthalpy conservation of Eq. (6), (7) on the assumption that constant-adiabatic process of combustion process.[1,2] In the main study, Kerosene and liquid oxygen was burned an equivalent ration of 1.4 in the 30 ton$_f$-class KARI LRE. It is used the inlet condition at nozzle flow analysis to obtain the combustor exit, pressure, temperature and elementally construction.

The chemical-equilibrium analysis of flow field achieved through the repetitive computing that obtain the temperature and pressure form Eq. (1) and then substitute these for Eq. (6), (7) and computing a chemical construction.

Flow analysis condition

A rocket engine, the 30 ton$_f$-class KARI LRE, is a area expansion ratio 60. The computing grid is used the 120×90 grid with clustering the nozzle wall and throat for the frozen and equilibrium flow computing, and apply a symmetry condition by an axis. The initial condition is given an adiabatic computing result of combustor on the whole domain. Moreover, the boundary condition used an adiabatic condition on the nozzle wall and the extrapolative subsonic condition on the inlet. Beside, the exit is given a lower pressure for the fast convergence on the early of computing. After, the extrapolative flow boundary condition is used in case of an exit mach 1. The initial and boundary condition are identically applied in the frozen and equilibrium.

Design conditions and performance analysis

Design conditions of LRE

The rocket engine considering in this study is 30 ton$_f$ - class KARI liquid rocket engine that has a expansion ratio of 60. The nozzle model used to this study has 120×90 grid points. The model is clustered to walls and throat. Elliptic smoothing method is applied to the model for verticality of grids. Axisymmetric nozzle model form is shown in Fig. 1.

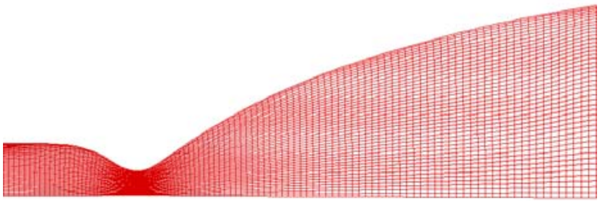


Fig. 1 Model of 30 ton$_f$ -class KARI LRE nozzle

Equilibrium analysis of combustion

The equilibrium analysis of combustion is performed for finding initial conditions of nozzle. The table 1 shows design conditions of the engine. The combustion chamber is assumed as constant pressure combustion. Adiabatic temperature of chamber is determined by enthalpy conservation equation. The table 2 shows results of equilibrium analysis and NASA CEA.

Table 1 Design specification of 30 ton$_f$ -class KARI LRE nozzle

Chamber Pressure	60 bar
Fuel	Jet – 60 ($C_{12}H_{23}$, 290 K)
Oxidizer	Liquid O_2 (90.17 K)
O/F Mass Ratio	2.44 (Φ =1.39)
Mass Flow Rate	88.8 kg/s
Throat Diameter	0.1805 m
Area Ratio	60

The Case 1 is considered the velocity on the enthalpy conservation equation after reaction and the case 2 is not considered that. Adiabatic temperature of case 1 is lower than that of case 2 as momentum energy by velocity. Errors of results are lower than that of 2 %. This study is considered 8 species in chemical mechanism, but CEA is considered 119 species. Functions and finding of equilibrium composition used to present study are also some different with CEA. Although some error exists in results of present code, the results have enough reliability.

Results of case 1 are used to initial and inlet conditions of nozzle.

Table 2 Temperature and species mole fraction in combustion

	Case 1	NASA CEA	Case 2
Temp. (K)	3618.12	3623.73	3629.57
H_2O	0.32304	0.31788	0.31644
CO_2	0.13535	0.13323	0.12288
CO	0.34402	0.34469	0.36195
OH	0.05005	0.05415	0.04402
O_2	0.01165	0.01179	0.00702
H_2	0.09694	0.09727	0.11110
O	0.00916	0.00944	0.00643
H	0.03077	0.03155	0.03013
U (m/s)	170.74	166.53	0

Nozzle performance

Thrust and specific impulse are generally defined as follows,

$$F = \dot{m} v_{exit} + \left(P_{exit} - P_{air}\right) A_{exit} \qquad (8)$$

$$I_{sp} = F / \dot{m} g \qquad (9)$$

The acceleration of gravity, *g* is 9.81 m/s^2. The velocity of exit is value of dividing total momentum flux into total mass rate. Pressure of exit is value dividing total force into total area.

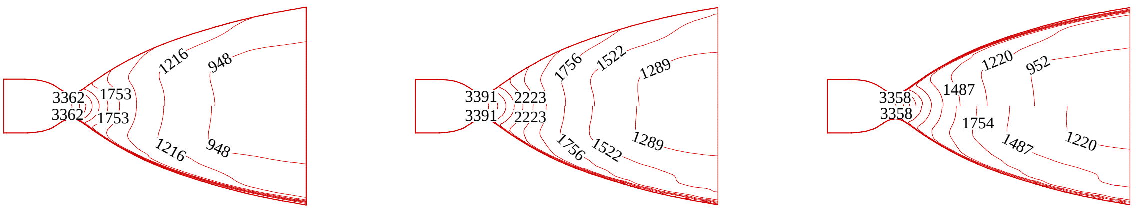
Results and Discussion

Thermal characteristics of nozzle flow

The Fig. 2 shows temperature distributions of each method in the nozzle. The difference of wall condition hardly affects to inner flow. In the non-slip condition, temperature variation of equilibrium analysis is lower than that of frozen flow analysis because the equilibrium flow is heated by recombination of chemical species.

The Fig. 3-5 show Mach number, pressure and velocity distributions in the nozzle. Although Mach number of frozen flow is higher than that of equilibrium flow, the exit velocity of equilibrium flow is higher than that of frozen flow by restoration of

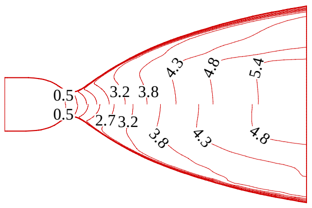
Frozen Equilibrium : Euler
Shifitng Equilibrium : Euler
Frozen Equilibrium : N.-S.



Frozen Equilibrium : N.-S.
Shifting Equilibrium : N.-S.
Shifting Equilibrium : N.-S.

Fig. 2 Temperature distributions in nozzle

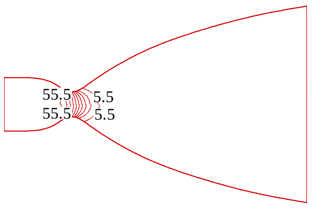
Frozen Equilibrium : N.-S.



Shifting Equilibrium : N.-S.

Fig. 3 Mach number distributions in nozzle

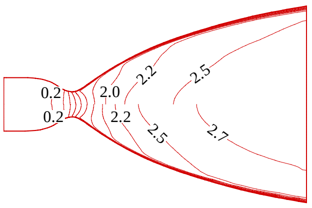
Frozen Equilibrium : N.-S.



Shifting Equilibrium : N.-S.

Fig. 4 Pressure distributions in nozzle

Frozen Equilibrium : N.-S.



Shifting Equilibrium : N.-S.

Fig. 5 Velocity distributions in nozzle

thermal energy.

The Fig. 6 shows distributions of vacuum thrust along area ratio by each method. The vacuum thrust represents the maximum thrust of nozzle in high altitude. The thrust performance of equilibrium analysis is higher than that of frozen analysis because of temperature difference. The results of wall slip conditions show high performance along area expansion ratio.

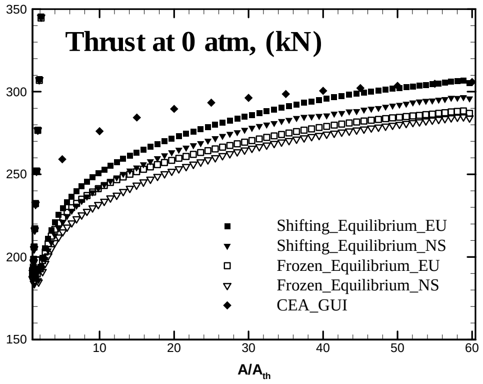


Fig. 6 Thrust distribution along area ratio at vacuum

The table 3 shows thrust performance according to each analysis in conditions of adiabatic and non-slip walls. The performance of NASA CEA is higher than other method because ideal equations are used to that. While results of frozen analysis show the minimum performance, those of equilibrium analysis show the maximum performance. The combustion efficiency is assumed 100%.

Table 3 Results of performance 30 ton_f-class KARI LRE nozzle

	Frozen Eq.	Shifting Eq.	NASA CEA	KARI Data
T (ton_f)	28.95	30.24	31.33	29.4
I_{sp} (s)	326.01	340.54	361.83	330

Conclusion

The performance limits of 30 ton_f-class KARI LRE nozzle and distribution of chemical species are estimated by equilibrium and frozen analysis. Although non-equilibrium analysis approaches real performance, it requires more time and computation resources than other method. Because the frozen and equilibrium analysis represent performance limits, the methods are made full use of the nozzle performance.

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