

# 跨音速喷管化学反应流数值模拟

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**【摘要】** 用时间相关的半隐格式有限差分数值方法求解了化学非平衡反应跨音速喷管流场, 在喷管收敛段, 流动接近化学平衡状态, 控制方程的刚性问题严重, 数值积分困难。通过对时间差分项隐式离散、对空间差分项显式离散, 流场边界采用参考平面上的特征线法计算等, 成功地解决了由于化学反应有限速率带来的数值解不稳定问题。该格式简单、需要计算机存储空间少。本文完成了一维和轴对称非平衡化学反应喷管流动计算, 并与化学平衡流和冻结流的计算结果做了比较。

主题词: 火箭发动机 喷管流动 数值模拟  
分类号: V435

## 1 前 言

火箭发动机工作过程中, 高温燃烧产物流经喷管, 由于化学反应速率是有限的, 各化学反应不可能跟随流动参数变化而时时处于化学平衡状态, 这就使喷管中的复合反应不完全, 造成化学动力学损失。预估发动机性能时, 要计算由于化学反应有限速率引起的化学动力学损失及其它损失。化学非平衡反应控制方程组中的组分连续方程是刚性(病态)方程, 如果用标准显式积分方法将存在严重的数值不稳定性。本文采用 Nakahashi 半隐格式<sup>[1]</sup>, 用时间相关法计算了一维和轴对称喷管流场。

## 2 控制方程和化学动力学模型

具有化学反应的可压、无粘、轴对称喷管流动在计算平面上的控制方程为:

$$\partial Z_i / \partial \tau = f_i \quad (i = 1, \cdots, N_s + 4) \quad (1)$$

其中  $Z_1 = \rho$ ,  $Z_2 = u$ ,  $Z_3 = v$ ,  $Z_4 = T$ ;  $z_{4+i} = Y_i$  ( $i = 1, \cdots, N_s$ )  
式中  $f_i$  是  $Z_i$  及其空间导数的函数;  $\tau$  为时间;  $u, v$  为轴向、径向速度;  $\rho, T$  为密度、温度;  $Y_i$  为组分  $i$  的质量分数;  $N_s$  为化学组分数目。计算平面上的坐标是  $\xi$  和  $\eta$ 。

控制方程中组分的净生成率  $\omega$  须由化学反应模型来确定。根据化学动力学理论, 基元反应方程式可写成一般形式:

$$\sum_{i=1}^{N_s} \nu_{ij} A_i \xrightleftharpoons[k_{bj}]{k_{fj}} \sum_{i=1}^{N_s} \nu'_{ij} A_i \quad (j = 1, \cdots, N_R) \quad (2)$$

式中  $\nu_{ij}, \nu'_{ij}$  为反应中反应物和生成物的化学计量系数;  $A_i$  为第  $i$  个组分,  $k_{fj}, k_{bj}$  为第  $j$  个反应的正向和逆向反应速率系数,  $N_R$  为基元反应数目。

考虑到基元反应中包含有只参与碰撞的中间体  $M$ , 由基元反应得组分  $i$  的净生成率为:

$$\omega = M_i \sum_{j=1}^{N_R} (v_j' - v_j) \left[ K_{fj} \prod_{k=1}^{N_s+1} \left( \frac{\rho Y_k}{M_k} \right)^{v_{kj}'} - K_{bj} \prod_{k=1}^{N_s+1} \left( \frac{\rho Y_k}{M_k} \right)^{v_{kj}} \right] \quad (3)$$

式中  $M_i$  是组分  $i$  的摩尔质量,  $k_{fj}$  由 Arrhenius 定律计算:

$$k_{fj} = A_j T^{\alpha_j} \exp(-E_j/R_0 T) \quad (4)$$

其中  $R_0$  是通用气体常数,  $E_j$  是第  $j$  个基元反应的正向反应的活化能,  $A_j$  和  $\alpha_j$  是常数, 与基元反应的正向反应有关。逆向反应速率常数  $k_{bj}$  由化学反应的平衡常数  $k_j$  来计算:

$$k_{bj} = k_{fj}/k_j \quad (5)$$

### 3 有限差分格式和边界条件

离散控制方程时, 对时间项作隐式差分, 而对空间项作显式差分, 应用时间二阶精度的 Crank-Nicolson 隐格式离散方程 (1), 得到

$$\Delta z_i^{n+1} = (\Delta \tau / 2) [f_i^n + f_i^{n+1}] \quad (i = 1, \cdots, N_s + 4) \quad (6)$$

式中  $\Delta z_i^{n+1} = z_i^{n+1} - z_i^n$ , 其中  $n, n+1$  是时间迭代步。方程 (6) 中的  $f_i^{n+1}$  是未知量  $z_j^{n+1} (j = 1, \cdots, N_s + 4)$  的非线性隐函数。为了求解  $z_i^{n+1}$ , 首先将  $f_i^{n+1}$  线性化, 把  $f_i$  看作是  $z_j, z_{\xi}, z_{\eta} (j = 1, \cdots, N_s + 4)$  的函数。用台劳级数展开, 得

$$f_i^{n+1} = f_i^n + \sum_{j=1}^{N_s+4} [A_{ij}^n \Delta z_j^{n+1} + B_{ij}^n \Delta z_{\xi_j}^{n+1} + C_{ij}^n \Delta z_{\eta_j}^{n+1}] \quad (7)$$

式中  $A_{ij} = \partial f_i / \partial z_j, B_{ij} = \partial f_i / \partial z_{\xi}, C_{ij} = \partial f_i / \partial z_{\eta}$ 。  $\Delta z_{\xi_j}^{n+1}$  和  $\Delta z_{\eta_j}^{n+1}$  按显式计算  $\Delta z_{\xi_j}^{n+1} = z_{\xi_j}^{n+1} - z_{\xi_j}^n = f_{\xi_j}^n \Delta \tau, \Delta z_{\eta_j}^{n+1} = z_{\eta_j}^{n+1} - z_{\eta_j}^n = f_{\eta_j}^n \Delta \tau$ 。由式 (6) 得

$$\Delta z_i^{n+1} - \frac{\Delta \tau}{2} \sum_{j=1}^{N_s+4} A_{ij}^n \Delta z_j^{n+1} = \frac{\Delta \tau}{2} (f_i^n + g_i^n) \quad (8)$$

式中  $g_i^n = f_i^n + \Delta \tau \sum_{j=1}^{N_s+4} [B_{ij}^n f_{\xi_j}^n + C_{ij}^n f_{\eta_j}^n]$ 。在流场中的每一节点求解该方程组, 就可得到  $n+1$  时间步的参数。为了使计算数值稳定, 对方程 (8) 中的  $f_i^n$  中的空间差分用两点后向差分, 而对  $A_{ij}^n, g_i^n$  中的空间差分用两点前向差分<sup>[1]</sup>。

入口边界: 采用  $\eta =$  常数的参考平面内的一个有效的相容性方程和给定喷管入口的流动角、总压、总温和各组分的质量分数 (按化学平衡流给出)。

壁面边界: 利用壁面边界条件和  $\xi =$  常数的参考平面内的  $N_s + 3$  个有效的相容性方程。

轴线边界: 沿轴线有  $v = 0$ , 其它  $N_s + 3$  个边界条件由轴对称条件来提供。

出口边界: 出口边界点的参数由相邻的 3 点外插得到。

### 4 算 例

喷管为收敛半角  $45^\circ$  扩张半角  $15^\circ$  喉部为圆弧的锥形喷管, 喉部圆弧半径和喷喉半径之比分别为 0.625 (喷管 1) 和 2 (喷管 2)。喷管收敛段面积比为 9.766, 扩张段面积比为 6.595。

#### 4.1 一维化学非平衡反应流计算

对于液氢—液氧推进剂的发动机, 表 1 列出了两种喷管型面在燃烧室压强为 3.43 MPa 下的真空比冲计算结果。热力计算的真空平衡比冲和冻结比冲也列于表 1。由表可见, 非平衡比冲介于平衡值和冻结值之间, 偏差在 3% 以内。喷管 1 型面在喉部的变化率较大, 流动参数也变化较快, 化学非平衡的影响明显, 其非平衡比冲与平衡比冲相差较大, 化学动力学损失较

表 1 化学非平衡真空比冲计算结果与热力计算结果的比较

|      | 平衡流(热计算) | 冻结流(热计算) | 非平衡流     | 偏差(平衡) | 偏差(冻结) |
|------|----------|----------|----------|--------|--------|
|      | N · s/kg | N · s/kg | N · s/kg | %      | %      |
| 喷管 1 | 3888.4   | 3720.3   | 3771.4   | - 3    | + 1.4  |
| 喷管 2 | 3888.4   | 3720.3   | 3826.4   | - 1.6  | + 2.8  |

大。图 1 示出了喷管 1 的无因次温度(燃气温度与喷管入口总温之比)分布。由图可见,化学反应流的温度介于化学平衡流和化学冻结流之间,而且在喷管的收敛段,流动接近化学平衡;在喉部及其下游,化学非平衡的影响逐渐显著,化学反应流的温度偏离化学平衡流。

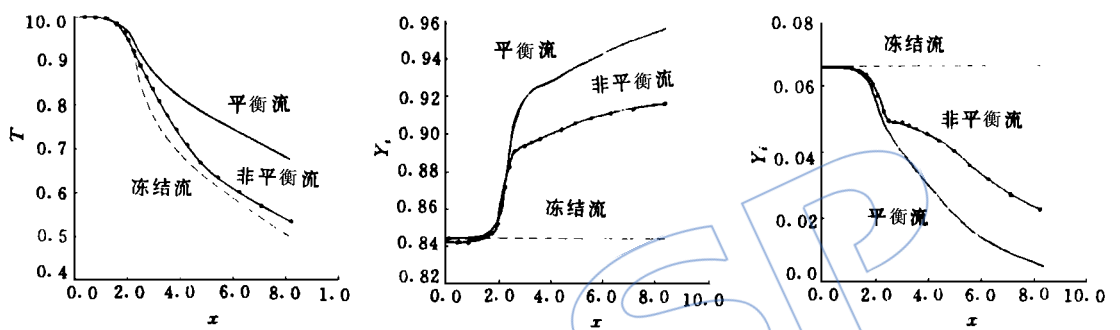


图 1 喷管 1 的无因次温度分布      图 2 喷管 1 中 H<sub>2</sub>O 的质量分数分布      图 3 喷管 1 中 OH 的质量分数分布

场中的 H<sub>2</sub>O、OH 的质量分数分布于图 2 和图 3。由图可见,在喉部上游的高温区,流动接近化学平衡,各组分基本保持化学平衡状态;以后,随着气体的膨胀,温度降低,复合反应占优势,因而, H<sub>2</sub>O 的质量分数增多, OH 和 H<sub>2</sub> 等的质量分数减少。与流动参数的分布一样,非平衡流的组分质量分数的分布介于化学平衡值和化学冻结值之间。

4.2 轴对称化学非平衡流计算

该计算的出口截面取在喷管喉部下游 1.5 倍喉部半径处。图 4 示出了喷管 2 壁上和轴上

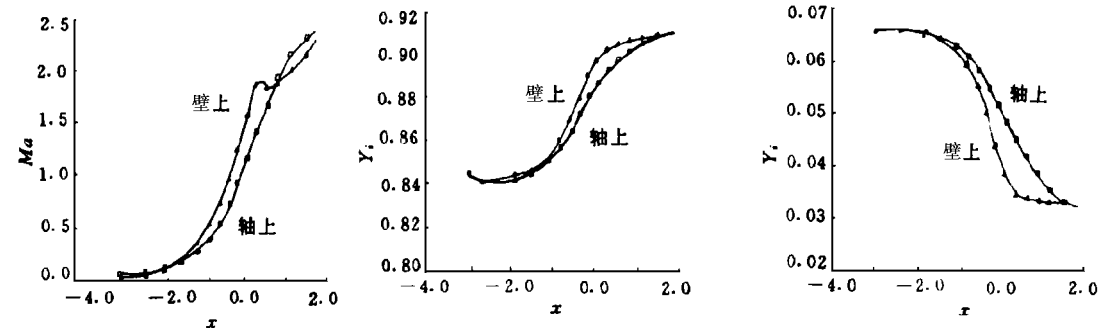


图 4 喷管 2 中壁上和轴上的马赫数分布      图 5 喷管 2 中壁上和轴上 H<sub>2</sub>O 的质量分数分布      图 6 喷管 2 中壁上和轴上 OH 的质量分数分布

的马赫数分布。由图可见, 化学反应流的流动参数分布曲线与无反应流的参数分布相似<sup>[2]</sup>。在喷管圆弧与扩张锥相切点附近, 由于壁面曲率半径不连续(即二阶导数不连续), 气流受压缩, 产生一道强压缩波。

图 5、图 6 分别示出喷管 2 壁上和轴上的  $\text{H}_2\text{O}$  和  $\text{OH}$  的质量分数分布。 $\text{H}_2\text{O}$  的质量分数随喷管中温度、压强降低而增加, 而  $\text{H}_2$  和  $\text{OH}$  都减小。这些结果符合化学动力学规律。

## 5 结 论

由于化学反应有限速率的影响, 在喷管收敛段, 流动接近于化学平衡, 化学反应流控制方程中的组分连续方程数值积分困难, 采用 Nakahashi 半隐格式能较好解决这一问题。本文完成的计算程序可作为预估喷管的化学动力学损失的基础和发动机工作过程仿真程序的一部分。本文只做了液氢—液氧推进剂系统的化学反应流动计算, 但该方法可推广到固体火箭发动机及其它推进系统(如超燃冲压发动机)的化学反应流计算。

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## FULL- LENGTH PAPERS

### NUMERICAL ANALYSIS OF THREE- DIMENSIONAL TURBULENT FLOW IN COMPRESSOR BLADE ROW BY IMPLICIT HIGH- RESOLUTION SCHEME

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#### ABSTRACT

It is found that a three or high order accurate high- resolution scheme may be more suitable for the correct prediction of turbulent flow field characteristics in the numerical analysis of three- dimensional turbulent shocked flow in transonic compressor blade row. The convergence of the three- dimensional turbulent flow calculation can be remarkably sped up by using the implicit LU- SGS algorithm, which is unconditionally stable. A detailed comparison between numerical solutions and experimental data indicates that their agreement is quite satisfactory.

**Key Words** Compressors High resolution Implicit methods Numerical simulation

### AN EXPERIMENT ON ENLARGING STEADY WORKING RANGE OF SKEWED- SWEEPED ROTATING BLADES

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#### ABSTRACT

An experimental investigation on enlarging the steady working range of skewed- swept rotating blades has been completed. Two types of fan were compared, a fan with conventional (radial) rotating blades and other with the skewed- swept blades. One comparative group was carried out on the conditions of same rotating speed and geometrical parameters but median chord of the skewed- swept rotating was increased about 20.4%, another was carried out at same peak pressure ratio and flow rate. The results of aerodynamic- aeroacoustic performance testing of the groups show not only a noise reduction about 2- 4 dB (A) overall, and an increase of aerodynamic efficiency for the skewed- swept blade, but also a great enlargement of steady working range (one group about 21%, other more than 22%). On the basis of the experimental results, the mechanism of the enlargement of steady working range for skewed- swept rotating blades was analyzed.

**Key Words** Blades Aerodynamic characteristics Acoustic properties Stability

### NUMERICAL SIMULATION OF REACTING FLOWS IN NOZZLE

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#### ABSTRACT

The numerical simulation of chemically reacting flows in the nozzle is accomplished by a time- dependent technique using semiimplicit scheme. A second- order implicit difference approximation is applied to the time derivatives in governing equations and a noncentered difference approximation is explicitly employed to the spatial derivatives. The numerical instability caused by the stiffness of chemical relaxation equations is successfully

depressed by the above measure. The results obtained from numerical simulation of one- dimensional and axisymmetric nozzle flows are presented.

**Key Words** Rocket engines Nozzle flow Numerical simulation

## NAVIER– STOKES PREDICTIONS OF 2– D VECTORED NOZZLE FLOWS

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### ABSTRACT

In this paper, the viscous flows in the two- dimensional vectored and unvectored nozzles are numerically simulated by three- dimensional time- dependent Navier– Stokes equations in conservation forms. Finite volume discretization is used in spatial form and Runge– Kutta method in time marching direction. A new viscous terms' discretization in the frame- work of the finite volume method is used which has the advantages of less operation counts and full conservation. A modified Baldwin– Lomax algebraic turbulent model and wall function law are also adopted in the prediction. Comparison of numerical predictions with experiments shows that the Navier– Stokes code can accurately predict the flow fields in the vectored and unvectored nozzle where the flow is predominantly two- dimensional at the designed nozzle pressure ratios or above. Discrepancies between predictions and experiment are found at lower nozzle pressure ratios where separation typically occurs in a large portion of the nozzle.

**Key Words** Jet nozzles Vector fields Numerical computation

## EFFECTS OF GEOMETRIC PARAMETERS OF SUBMERGED DELTA VORTEX GENERATOR ON VORTEX

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### ABSTRACT

The effects of the geometric variables of a submerged deltaic vortex generator on the parameters of the vortex have been experimentally studied and a type of half deltaic vortex generator has been developed. A small- size five- hole pressure probe was used to measure the velocity profiles at several transverse sections behind the vortex generators and according to the velocity profiles, the Gauss model of vortex core and quasi- Newton non- linear least square method were used to determine the parameters of single vortex such as vorticity, radius and height of the vortex core. The variation of these vortex parameters along the stream wise was analysed. In the experimental investigation the vortex parameters between the submerged deltaic vortex generator and the submerged concave vortex generator were also compared.

**Key Words** Swirler Velocity distribution Geometric parameters Vortex

## EFFECTS OF AUTOMATICALLY POSITIONING BLADE ON FLOW CHARACTERISTICS IN AN S– SHAPED AIR INLET

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### ABSTRACT

An automatically positioning blade with a NACA 0012- series profile was placed upstream near the throat of an S- shaped diffuser and experimented to investigate the characteristics of the flow behind it. The results show that two angular positions have been found where the blade experiences no resultant aerodynamic moment, i. e.  $15^\circ$  and