

AUPOIX B., SPALART; P. R. Extensions of the Spalart – Allmaras turbulence model to account for wall roughness. International Journal of Heat and Fluid Flow. Vol 24, pp 454 – 462, 2003.

BATINA, J. Implicit flux-split Euler schemes for unsteady aerodynamic analysis involving unstructured dynamic meshes. American Institute of Aeronautics and Astronautics Journal, 29:1836, 1991.

BOURGOYNE, A. T.; MILHEIM, K. K.; CHENEVERT, M. E.; YOUNG, F. S. Applied Drilling Engineering. Society of Petroleum Engineers, 1991.

BROWNING, J. A. Flame-Jet Drilling in Conway, N. H. Granite. Unpublished report, University of California, 1981.

BROWNING, J. A., et al. Recent Advances in Flame Jet Working of Minerals. 7th Symposium on Rock Mechanics, Pennsylvania State University, 1965.

CALAMAN, J. J.; ROLSETH, H. C. Technical Advances Expand Use of Jet-Piercing Process in Taconite Industry. International Symposium on Mining Resources, University of Missouri, 1961.

DEY, T. N. More on spallation theory. Los Alamos National Laboratory Internal Memorandum No ESS-3-286-84, 1984.

DEY, T. N.; KRANZ, R. L. Methods for Increasing Drilling Performance of the Thermal Spallation Drilling System. 9th Conference of Geothermal Resources Council, 1985.

FIGUEIRA DA SILVA, L. F.; AZEVEDO, J.; KORZENOWSKI, H. Unstructured adaptive grid flow simulations of inert and reactive gas mixture. J. Comput. Phys, Vol. 160 No. 2 pp. 522 – 540, 2000.

FIGUEIRA DA SILVA, L. F.; NIECKELE, O. A.; SALGADO, F.; PLÁCIDO, J. C. Numerical study of the flowfield structures during thermal spallation drilling process. In 10TH Brazilian congress of thermal sciences and engineering, Rio de Janeiro, Brazil, 2004.

GLAZNEV, V. Inverse feedback mechanism in self-oscillations in flow of an underexpanded supersonic jet against a planar obstacle. Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, (transl.), Vol. 4, pp. 59 – 63, 1991.

GORSHKOV, G. F.; USKOV, V. Special features of self-sustained oscillations in a supersonic underexpanded jet impinging on an obstacle with a restricted cross-section. Prikladnaya Mekhanika i Tekhicheskaya Fizika, (transl.), Vol. 40, pp. 143 – 149, 1999.

GORSHKOV, G. F.; USKOV, V. N.; FAVORSKII, V. S. Nonstationary flow of an underexpanded jet around an unbounded obstacle. Prikladnaya Mekhanika i Tekhicheskaya Fizika, (transl.), Vol. 4, pp. 58 – 65, 1993.

HIRSCH, C. Numerical Computation of Internal and External Flows, John Wiley & Sons, 1990.

[Http://www.geocities.com.br](http://www.geocities.com.br)

JIAN, S. S. Upwind Differencing and LU Factorization for Chemical Non – equilibrium Navier – Stokes Equations. Journal of Computational Physics, Vol. 99, pp. 233 – 250, 1992.

LIU, M – S. A Sequel to AUSM: AUSM⁺. Journal of Computational Physics, Vol. 129, No. 2, pp. 364 – 382, 1996.

MARQUES, A. N.; SIMÕES, C. F.; AZEVEDO, J. L. Unsteady Aerodynamic Forces for Aeroelastic Analysis of Two – Dimensional Lifting Surfaces. Journal of the Brazilian. Society . of Mechanical. Science and Engineers , Vol. 28, No. 4, pp. 475 – 485, 2006.

MILITKÝ, J.; KOVACIC, V.; RUBNEROVA, J. Influence of thermal treatment on tensile failure of basalt fibers. Engineering. Fracture Mech., Vol. 69, pp. 1025 – 1033, 2002.

PANDA, J. Shock oscillation in underexpanded screeching jets. J. Fluid Mech, Vol. 363, pp.173 -198, 1998.

PENG, S.; JOHNSON, A. M. Crack growth and faulting in cylindrical specimens of Chelmsford granite. International Journal of Rock Mechanics and Mining Sciences, v. 9, n. 1, p. 37-86, 1972.

POINSOT, T. J., LELE, S. K. Boundary conditions for direct simulations of compressible viscous flows. Journal of Computational physics, Vol. 101, No. 104 – 129, 1992.

PRESTON, F. W. Observations on Spalling. *Journal of the American Ceramic Society* 17: 137-144, 1934.

RAUENZAHN, R. Analysis of rock mechanics and gas dynamics of flame-jet thermal spallation drilling. Ph.D. Thesis, Massachusetts Institute of Technology, 1986a.

RAUENZAHN, R.; TESTER, J. Rock Failure Mechanisms of Flame-Jet Thermal Spallation Drilling – Theory and Experimental Testing. *International Journal of Rock Mechanics and Mining Sciences & Geomechanics Abstracts*, Vol. 26, No. 5, pp. 381 – 399, 1986b.

RAUENZAHN, R. M.; TESTER, J. Numerical simulation and field testing of flame-jet thermal spallation drilling. 1. Experimental verification. “*International Journal of Heat Mass Transfer*”, Vol. 34, No. 3, pp. 795 – 808, 1991.

RODRIGUES, F. J.; BASTOS, D.; FIGUEIRA DA SILVA, L. F.; PLÁCIDO, J. C. Analysis of the performance of a thermal spallation device for rock drilling. 11th Brazilian congress of thermal Sciences and Engineering. 2006.

SALGADO, F. Estudo numérico das estruturas do escoamento de perfuração por descamação térmica (Thermal Spallation Drilling). Projeto de graduação Engenharia Mecânica, 2005.

SARKAR, S.; ERLEBACHER, G.; HUSSAINI, M. Y.; KREISS, H. O. The analysis and modeling of dilatational terms in compressible turbulence. *J. Fluid Mech.*, Vol. 227, pp. 473 – 493, 1991.

SCHLICHTING, H. *Boundary – Layer Theory*, 8th ed. McGraw-Hill, New York, 2000.

SIMÕES, C.; AZEVEDO, J. Unsteady airfoil inviscid flow simulation using unstructured dynamics mesh. XIV Brazilian Congress of Mechanical Engineers, 1997.

SOKOLOV, E. Breakdown of steady axisymmetric flow in the shock layer formed when a supersonic underexpand jet interacts with a perpendicular flat plate. *Izvestiya Rossikoi Akademii Nauk, Mekhanika Zhidkosti Gaza*, (transl.), Vol. 4, pp. 36 – 42, 1992.

SPALART P. R.; ALLMARAS, S. R. A one-equation turbulence for aerodynamics flows. *La Recherche Aéronautique*, No. 1, pp 5 – 21, 1994.

STRAUSS, D.; AZEVEDO, J. L. Unstructured multigrid simulations of turbulent launch vehicle flows including a propulsive jet. In: 20TH AIAA APPLIED AERODYNAMICS CONFERENCE, 2002.

TESTER, J. W.; HERZOG, Z.; CHEN, R. M.; POTTER; FRANK, M. G. Prospects for Universal Geothermal Energy from Heat Mining. Science & Global Security, Vol. 5, pp. 99 – 121, 1994.

TESTER, J. W. et al, The Future of Geothermal Energy, An assessment by an MIT-led interdisciplinary panel, pp 1 – 372, 2006.

WALTER, M. A. T.; ABDU, A. A. Q.; FIGUEIRA DA SILVA, L. F.; AZEVEDO, J. L. Evaluation of adaptive mesh refinement and coarsening for the computation of compressible flows on unstructured meshes. International Journal for Numerical Methods in Fluids, Vol. 49, pp. 999 – 1014, 2005.

WEIBULL, W. A Statistical Theory of the Strength of Materials. Engineers. Vetenskaps Akad. Handl. 151: 1-45, 1939.

WILLIAMS, F. A. Combustion Theory, Benjamin/Cummings Publishing Company, Inc., second edition, 1985.

WILLIAMS, R. E.; DEY, T.; RAUENZANH, R.; KRANZ, R.; TESTER, J.; POTTER, R.; MURPHY, H. Advancements in thermal spallation drilling technology. Los Alamos, N.M.: Los Alamos National Laboratory. (LA-11391-MS), 1988.

WILKINSON, M. A. Computational Modeling of the Gas-Phase Transport Phenomena and Experimental Investigation of Surface Temperature During Flame-Jet Thermal Spallation Drilling. Ph.D Thesis, Department of Chemical Engineering, Massachusetts Institute of Technology: 273, 1989.

WILKINSON, M.; TESTER, J. Experimental Measurement of Surface Temperatures During Flame-Jet Induced Thermal Spallation Drilling, Rock Mechanics and Rock Engineering, Vol. 26, No. 1, pp. 29 – 62., 1993a.

WILKINSON, M.; TESTER, J. Computational modeling of the gas-phase transport phenomena during flame-jet thermal spallation drilling. International Journal of Heat Mass Transfer, Vol. 36, No. 14, pp. 3459 – 3475, 1993b.

ZEMAN, O. A new model for super/hypersonic turbulent boundary layers. In 31st Aerospace Science Meeting & Exhibit, (AIAA Paper 93-0897), 1993.

ZHANG, H. S.; SO, R. M.; SPEZIALE, C. G.; LAI, Y. G. A near-wall two-equation model for compressible turbulent flows. NASA Contractor Report 1895565 e ICASE Report., pp. 91 – 28, 1991.

Anexo A

As condições de contorno de entrada e de saída foram analisadas levando em conta os conceitos das equações características, estas equações são utilizadas no desenvolvimento de escoamentos compressíveis, já que neste tipo de escoamentos, as condições de entrada e de saída não podem ser tratadas da mesma forma que um escoamento incompressível, pela variação das propriedades.

Este anexo contém a dedução analítica das condições de contorno na entrada e na saída do bocal, que foram implementadas no código BRU2D, tais condições estão baseadas nas matrizes dos auto vetores pela direita e pela esquerda desenvolvidas por Shuen (1992). Na análise destas condições a velocidade é um problema bidimensional, pela propagação do escoamento, já que este é tem a forma de linhas de corrente as quais são analisadas pela equação da hipérbole.

Matriz S

$$S := \begin{bmatrix} 1 & 0 & \frac{\rho \sqrt{2}}{2a} & \frac{\rho \sqrt{2}}{2a} & 0 \\ u & 0 & \frac{\rho (u+a) \sqrt{2}}{2a} & \frac{\rho (u-a) \sqrt{2}}{2a} & 0 \\ v & -\rho & \frac{\rho v \sqrt{2}}{2a} & \frac{\rho v \sqrt{2}}{2a} & 0 \\ H - \frac{\rho a^2}{p_e} & -\rho v & \frac{\rho (H+ua) \sqrt{2}}{2a} & \frac{\rho (H-ua) \sqrt{2}}{2a} & -\frac{\rho^2 p_{ci}}{p_e} \\ Y_i & 0 & \frac{\rho Y_i \sqrt{2}}{2a} & \frac{\rho Y_i \sqrt{2}}{2a} & \rho \end{bmatrix}$$

Inversa da matriz S,

$$InverS := \begin{bmatrix} 1 - \frac{\phi}{a^2} & \frac{u p_e}{\rho a^2} & \frac{v p_e}{\rho a^2} & -\frac{p_e}{\rho a^2} & -\frac{p_{ci}}{a^2} \\ \frac{v}{\rho} & 0 & -\frac{1}{\rho} & 0 & 0 \\ \frac{\sqrt{2}(-u a + \phi)}{2 \rho a} & \frac{\sqrt{2}\left(a - \frac{u p_e}{\rho}\right)}{2 \rho a} & -\frac{\sqrt{2} v p_e}{2 \rho^2 a} & \frac{\sqrt{2} p_e}{2 \rho^2 a} & \frac{p_{ci} \sqrt{2}}{2 \rho a} \\ \frac{\sqrt{2}(u a + \phi)}{2 \rho a} & -\frac{\sqrt{2}\left(a + \frac{u p_e}{\rho}\right)}{2 \rho a} & -\frac{\sqrt{2} v p_e}{2 \rho^2 a} & \frac{\sqrt{2} p_e}{2 \rho^2 a} & \frac{p_{ci} \sqrt{2}}{2 \rho a} \\ -\frac{y_i}{\rho} & 0 & 0 & 0 & \frac{1}{\rho} \end{bmatrix}$$

onde o valor de ϕ , a^2 que se encontra nas matrizes anteriores, estão dadas nas equações. A.1 e A.2, respectivamente, para facilitar a análise das equações características.

$$\phi = p_\rho + \frac{p p_e}{\rho^2} - \frac{p_e}{\rho} (H - u^2 - v^2), \quad (A.1)$$

$$a^2 = p_\rho + \frac{p_e p}{\rho^2} + \sum y_i p_{ci}, \quad (A.2)$$

sendo c_i a concentração de massa das espécies químicas dada por,

$$c_i = \rho y_i, \quad (A.3)$$

Na eq. A.1 tem-se H que é a equação de transporte, que esta dada por:

$$H = \mathbf{e}_t + \frac{p}{\rho}, \quad (\text{A.4})$$

Para obter as equações características $l_i, i = 1, \dots, 3 + I$ deve proceder-se da seguinte maneira:

$$l = \begin{bmatrix} u \\ v \\ u + a \\ u - a \\ \vdots \\ u \\ \vdots \end{bmatrix} S^{-1} \frac{\partial \rho \psi}{\partial n}, \quad \psi = (1, u, v, \mathbf{e}_t, \dots, y_i) \quad (\text{A.5})$$

n é a direção normal à face considerada, u e v são as componentes da velocidade normal e paralela à face, respectivamente, assim pode-se escrever os l_i .

Substituindo a inversa da matriz S na equação A.5 são definidas as equações características,

$$l_1 = u \left[\left(1 - \frac{\phi}{a^2} \right) \frac{\partial \rho}{\partial n} + \frac{p_e}{\rho a^2} \left(u \frac{\partial \rho u}{\partial n} + v \frac{\partial \rho v}{\partial n} - \frac{\partial \rho \mathbf{e}_t}{\partial n} \right) - \sum_{i=1}^{I-1} \frac{p_{ci}}{a^2} \frac{\partial \rho y_i}{\partial n} \right], \quad (\text{A.6})$$

$$l_2 = u \left[\frac{v}{\rho} \frac{\partial \rho}{\partial n} - \frac{1}{\rho} \frac{\partial \rho v}{\partial n} \right], \quad (\text{A.7})$$

$$l_3 = \frac{u + a}{\sqrt{2\rho a}} \left[(-ua + \phi) \frac{\partial \rho}{\partial n} + \left(a - \frac{up_e}{\rho} \right) \frac{\partial \rho u}{\partial n} - \frac{vp_e}{\rho} \frac{\partial \rho v}{\partial n} + \frac{p_e}{\rho} \frac{\partial \rho \mathbf{e}_t}{\partial n} + \sum_{i=1}^{I-1} p_{ci} \frac{\partial \rho y_i}{\partial n} \right], \quad (\text{A.8})$$

$$l_4 = \frac{u - a}{\sqrt{2\rho a}} \left[(ua + \phi) \frac{\partial \rho}{\partial n} - \left(a + \frac{up_e}{\rho} \right) \frac{\partial \rho u}{\partial n} - \frac{vp_e}{\rho} \frac{\partial \rho v}{\partial n} + \frac{p_e}{\rho} \frac{\partial \rho \mathbf{e}_t}{\partial n} + \sum_{i=1}^{I-1} p_{ci} \frac{\partial \rho y_i}{\partial n} \right], \quad (\text{A.9})$$

resolvendo as equações A.6, A.7, A.8, A.9 se obtém as expressões finais para equações características:

$$l_1 = u \left(\frac{\partial \rho}{\partial n} - \frac{1}{a^2} \frac{\partial p}{\partial n} \right) \quad (\text{A.10})$$

$$l_2 = -u \frac{\partial v}{\partial n}, \quad (\text{A.11})$$

$$l_3 = \frac{u+a}{\sqrt{2}} \left[\frac{\partial u}{\partial n} + \frac{1}{a\rho} \frac{\partial p}{\partial n} \right] \quad (\text{A.12})$$

$$l_4 = \frac{u-a}{\sqrt{2}} \left[\frac{1}{a\rho} \frac{\partial p}{\partial n} - \frac{\partial u}{\partial n} \right] \quad (\text{A.13})$$

O calculo destas equações características são baseadas no trabalho feito por Thompson (1987), no qual para o desenvolvimento de casos unidimensionais e bidimensionais, a equação da energia é resolvida usando aproximações de diferenças finitas para derivadas espaciais, e a solução de uma equação diferencial ordinária explícita, para a integração das derivadas respeito ao tempo das variáveis conservativas; além disso, foi utilizada a inversa da matriz S dos auto vetores do trabalho feito por Shuen (1992), onde esta matriz é usada freqüentemente na função de fluxos numéricos.

Substituindo as equações características nas equações governantes (vide capítulo 3), são determinadas as condições de contorno na entrada e na saída do bocal, levando em conta a direção da propagação das características através da face.

$$\frac{\partial \rho}{\partial t} + l_1 + \frac{\rho}{\sqrt{2}a} (l_3 + l_4) = 0, \quad (\text{A.14})$$

$$\frac{\partial \rho u}{\partial t} + u l_1 + \frac{\rho u}{\sqrt{2}a} (l_3 + l_4) + \frac{\rho}{\sqrt{2}} (l_3 - l_4) = \frac{\partial \rho u}{\partial t} - u \frac{\partial \rho}{\partial t} + \frac{\rho}{\sqrt{2}} (l_3 - l_4) = 0 \quad (\text{A.15})$$

$$\frac{\partial \rho v}{\partial t} + v l_1 - \rho l_2 + \frac{\rho v}{\sqrt{2a}} (l_3 + l_4) = \frac{\partial \rho v}{\partial t} - v \frac{\partial \rho}{\partial t} - \rho l_2 = 0 \quad (\text{A.16})$$

$$\frac{\partial \rho e_t}{\partial t} + \left(H - \frac{\rho a^2}{p_e} \right) l_1 - \rho v l_2 + \frac{\rho H}{\sqrt{2a}} (l_3 + l_4) + \frac{\rho u}{\sqrt{2}} (l_3 - l_4) - \frac{\rho^2}{p_e} \sum_{i=1}^{I-1} p_{ci} l_{i+4} = 0 \quad (\text{A.17})$$

$$\frac{\partial \rho y_i}{\partial t} + y_i l_1 + \frac{\rho y_i}{\sqrt{2a}} (l_3 + l_4) + \rho l_{i+4} = \frac{\partial \rho y_i}{\partial t} - y_i \frac{\partial \rho}{\partial t} + \rho l_{i+4} = 0 \quad (\text{A.18})$$

- ❖ Considerando o fluxo subsônico na entrada, se tem que a densidade ρ e y_i que é a concentração de massa das espécies i são invariáveis no tempo. As demais variáveis são constantes.

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho y_i}{\partial t} = 0, \quad l_{i+4} = 0 \quad (\text{A.19})$$

Substituindo a eq. A.19 na eq. A.14 tem-se:

$$l_1 = -\frac{\rho}{\sqrt{2a}} (l_3 + l_4) \quad (\text{A.20})$$

Se $\frac{u}{v}$ e conhecido, e $\frac{\partial \rho e_t}{\partial t} = 0$ (pela razão de velocidade), então da eq.

A.17,

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho y_i}{\partial t} = \frac{\partial \rho v}{\partial t} = \frac{\partial \rho u}{\partial t} = 0, \quad l_2 = 0 \quad (\text{A.21})$$

$$\left(H - \frac{\rho a^2}{p_e} \right) l_1 + \frac{\rho H}{\sqrt{2a}} (l_3 + l_4) + \frac{\rho u}{\sqrt{2}} (l_3 - l_4) = 0 \quad (\text{A.22})$$

Da eq. A.16 e A.18 tem-se que,

$$\begin{aligned}
& \left(H - \frac{\rho a^2}{p_e} \right) \left[-\frac{\rho}{\sqrt{2}a} (l_3 + l_4) \right] + \frac{\rho H}{\sqrt{2}a} (l_3 + l_4) + \frac{\rho u}{\sqrt{2}} (l_3 - l_4) = 0 \\
& \frac{\rho_2}{\sqrt{2}p_e} (l_3 + l_4) + \frac{\rho u}{\sqrt{2}} (l_3 - l_4) = 0 \\
& (l_3 + l_4) + \frac{Mp_e}{\rho} (l_3 + l_4) = 0 \\
& l_3 \left(1 + \frac{Mp_e}{\rho} \right) + l_4 \left(1 - \frac{Mp_e}{\rho} \right) = 0 \quad \frac{p_e}{\rho} = \gamma - 1
\end{aligned} \tag{A.23}$$

$$l_3 = \left[\frac{M(\gamma - 1) - 1}{1 + M(\gamma - 1)} \right] l_4, \tag{A.24}$$

Agora,

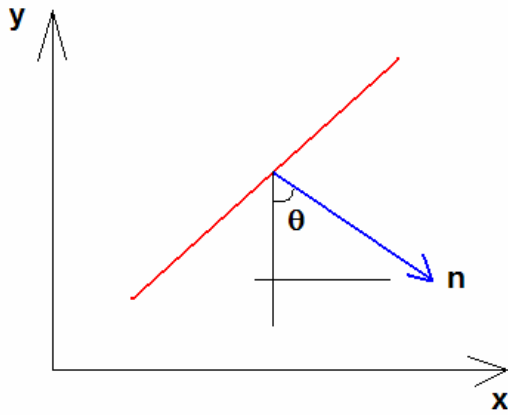
$$\begin{aligned}
& \frac{\partial \rho u}{\partial t} - \frac{\partial \rho}{\partial t} + \frac{\rho}{\sqrt{2}} (l_3 - l_4) = 0 \\
& \frac{\partial \rho u}{\partial t} = -\frac{\rho}{\sqrt{2}} (l_3 - l_4)
\end{aligned} \tag{A.25}$$

$$\frac{\partial \rho u}{\partial t} = \frac{\rho l_4}{\sqrt{2}} \left[1 - \frac{M \left(\frac{p_e}{\rho} \right) + 1}{1 + M \left(\frac{p_e}{\rho} \right)} \right] \quad \frac{p_e}{\rho} = \gamma - 1,$$

$$\frac{\partial \rho u}{\partial t} = \left[\frac{2}{1 + M(\gamma - 1)} \right] \frac{\rho}{\sqrt{2}} l_4. \tag{A.26}$$

- ❖ Análise para a saída para um fluxo subsônico, os valores próprios das características entrantes de $(u_n - a)$ é ajustada a zero. As demais características são calculadas do interior do campo do fluxo.

Com $l_4 = 0$,



Calculo dos cossenos diretores da velocidade levando em conta a direção do escoamento,

$$\begin{aligned} \frac{\Delta x}{\Delta n} &= \sin \theta = S_x & u_n &= S_x u - S_y v \\ \frac{\Delta y}{\Delta n} &= -\cos \theta = -S_y & u_t &= S_y u + S_x v \end{aligned} \quad (\text{A.27})$$

$$\frac{\partial \rho u}{\partial t} = S_x \frac{\partial u_n}{\partial t} + S_y \frac{\partial \rho u_t}{\partial t}, \quad (\text{A.28})$$

$$\frac{\partial \rho u}{\partial t} = (S_x u + S_y v) \frac{\partial \rho}{\partial t} + \rho \left(S_y l_2 - \frac{l_3}{\sqrt{2}} S_x \right), \quad (\text{A.29})$$

$$\frac{\partial \rho v}{\partial t} = (S_x v - S_y u) \frac{\partial \rho}{\partial t} + \rho \left(S_x l_2 + \frac{l_3}{\sqrt{2}} S_y \right), \quad (\text{A.30})$$

Pela transformada se calcula as derivadas da velocidade normal e tangencial à face, sendo ela um problema bidimensional.

$$\frac{\partial \rho u_n}{\partial t} = S_x^2 \frac{\partial u}{\partial x} - S_x S_y \frac{\partial u}{\partial y} - S_x S_y \frac{\partial v}{\partial x} + S_y^2 \frac{\partial v}{\partial y}, \quad (\text{A.31})$$

$$\frac{\partial \rho u_t}{\partial t} = S_x^2 \frac{\partial v}{\partial x} + S_x S_y \frac{\partial u}{\partial x} - S_x S_y \frac{\partial v}{\partial y} - S_y^2 \frac{\partial u}{\partial y}, \quad (\text{A.32})$$

com a equação de estado tem-se que:

$$p = \rho RT \sum \frac{y_i}{w_i}, \quad (\text{A.33})$$

$$\frac{\partial p}{\partial n} = \frac{RT}{\bar{W}} \frac{\partial \rho}{\partial n} + \frac{\rho R}{\bar{W}} \frac{\partial T}{\partial n} + \rho RT \sum \frac{1}{w_i} \frac{\partial y_i}{\partial n}, \quad (\text{A.34})$$

$$\frac{\partial \rho}{\partial n} = \frac{\bar{W}}{RT} \frac{\partial p}{\partial n} - \frac{\rho}{T} \frac{\partial T}{\partial n} - \bar{W} \rho \sum \frac{1}{w_i} \frac{\partial y_i}{\partial n} \quad \dots\dots \quad \frac{\bar{W}}{RT} = \frac{\rho}{p}, \quad (\text{A.35})$$

$$\frac{\partial \rho}{\partial n} = \frac{\rho}{p} \frac{\partial p}{\partial n} - \frac{\rho}{T} \frac{\partial T}{\partial n} - \bar{W} \rho \sum \frac{1}{w_i} \frac{\partial y_i}{\partial n}, \quad (\text{A.36})$$

$$\frac{1}{\rho} \frac{\partial \rho}{\partial n} = \frac{1}{p} \frac{\partial p}{\partial n} - \frac{\rho}{T} \frac{\partial T}{\partial n} - \bar{W} \sum \frac{1}{w_i} \frac{\partial y_i}{\partial n} \quad . \quad (\text{A.37})$$