

The details of the derivation are given in Ref. 5. Note that if both  $k_x$  and  $k_z$  are zero, certain coefficients are then undefined. This condition is easily remedied by choosing to rotate the given  $[k_x/D, k_y/D, k_z/D]$  vector to the "closest" unit axis vector ( $x, y$ , or  $z$ ). This practice will ensure a nonzero denominator in the expressions for the coefficients  $c_i$ . (The above expressions are derived by rotating the  $[k_x/D, k_y/D, k_z/D]$  vector to a unit vector on the  $x$  axis.)

Excluding a redefinition of the invariants  $\hat{v}$  and  $\hat{w}$  by either of the methods presented in this Note, there are no other required changes to the Osher algorithm for use in general computations. The reader is then referred to Ref. 4 for a more detailed description of the scheme.

### References

- <sup>1</sup>Chakravarthy, S. R. and Osher, S., "Numerical Experiments with the Osher Upwind Scheme for the Euler Equations," AIAA Paper 82-0975, June 1982.
- <sup>2</sup>Chakravarthy, S. R. and Osher, S., "High Resolution Applications of the Osher Upwind Scheme for the Euler Equations," AIAA Paper 83-1943, June 1983.
- <sup>3</sup>Rai, M. M. and Chakravarthy, S. R., "An Implicit Form for the Osher Upwind Scheme," *AIAA Journal*, Vol. 24, May 1986, pp. 735-743.
- <sup>4</sup>Osher, S. and Chakravarthy, S., "Upwind Schemes and Boundary Conditions with Applications to Euler Equations in General Geometries," *Journal of Computational Physics*, Vol. 50, 1983, pp. 447-481.
- <sup>5</sup>Hesseniuss, K. and Rai, M. M., "Three-Dimensional, Conservative, Euler Computations using Patched Grid Systems and Explicit Methods," AIAA Paper 86-1081, May 1986.
- <sup>6</sup>Rogers, S., Chang, J., and Kwak, D., "A Diagonal Algorithm for the Method of Pseudocompressibility," AIAA Paper 86-1060, May 1986.

## Entropy Production in Nonsteady General Coordinates

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### Introduction

THE second law of thermodynamics is generally not utilized in CFD algorithms, since the law is not essential for obtaining a flowfield solution. However, there are circumstances where the relevance of the second law should not be overlooked. These occur in flows where the entropy production by natural (i.e., irreversible) processes is large, e.g., a chemically reacting boundary layer. For a valid solution, entropy production caused by the algorithm or numerical processes should be small in comparison. There are a variety of sources for numerically produced entropy, including artificial viscosity or damping terms, round-off and truncation errors, and numerical instabilities.

It has become common practice to compute a steady-flow solution by using the nonsteady equations of motion. During the lengthy nonsteady computation, the numerically produced entropy may gradually accumulate. The validity of the computation is then uncertain unless this entropy production, at termination, is still small in comparison to that produced by natural processes.

As an illustration, we have in mind two interesting studies. Both used the nonsteady, conical, Euler equations to asymptotically obtain steady-flow results. (We do not suggest by these remarks that either study is suspect.) One study<sup>1</sup> examined the stability of shock waves attached to wedges or cones. The other<sup>2</sup> examined the large total pressure loss in a vortical flow on the leeward surface of a swept wing. Entropy production by natural processes is significant in both flows. Nevertheless, it would be useful to know the numerically produced contribution.

As a first step, of course, we need to establish the entropy production of the natural processes. This Note addresses this subject. The determination, however, is not a straightforward task, in part, because the second law is usually formulated as an inequality. This difficulty is avoided by focusing on the rate of entropy production.<sup>3,4</sup> Because of the complexity of real flows, CFD algorithms often use nonsteady, general, boundary-fitted coordinates. A number of recent publications<sup>5-7</sup> have discussed the conservation equations when written in this type of coordinate system. As a supplement to these references, we derive the second law in a corresponding form.

For the purposes of generality, a variety of processes are considered. These include conductive and radiative heat transfer, viscous dissipation, chemical reactions, and molecular diffusion. In the first part of the analysis, the thermodynamic equations are formulated in an invariant form. In the final section, an equation is obtained in the aforementioned coordinate system for the rate of entropy production. This equation is our principle result.

### Thermodynamics

A Newtonian fluid in a continuum flow is assumed. The energy equation can be written as<sup>3</sup>

$$\rho \frac{Dh}{Dt} - \frac{Dp}{Dt} = -\text{div}(q_E + q_R) + \Phi \quad (1)$$

where  $D/Dt$  is the substantial derivative,  $\rho$  the density, and  $p$  the pressure. The specific enthalpy  $h$  contains<sup>3</sup> the radiative energy density  $u_R$ , while the pressure similarly contains a contribution from the radiative stress tensor. Both contributions are almost always negligible<sup>8</sup> and we neglect these terms in the rest of the discussion. The energy-diffusion flux and radiative heat flux for a mixture of  $N$  thermally perfect gases are given by

$$q_E = -k \text{grad } T + \sum_{\alpha=1}^N h_{\alpha} j_{\alpha}$$

$$q_R = \int_0^{\infty} \int_0^{4\pi} I_{\nu} \hat{I} d\Omega d\nu \quad (2)$$

where  $k$  is the thermal conductivity,  $T$  the temperature, and  $h_{\alpha}$  the specific enthalpy of species  $\alpha$ . A lengthy constitutive equation for the mass-diffusion flux vector for species  $\alpha$ ,  $j_{\alpha}$ , can be found in Ref. 9. In Eq. (2),  $I_{\nu}$  is the radiative specific intensity at frequency  $\nu$  in a differential solid angle  $d\Omega$  and the unit vector  $\hat{I}$  specifies the direction of propagation of  $I_{\nu}$ .

The viscous dissipation function  $\Phi$  in Eq. (1) is the double-dot product of the stress tensor  $\vec{\tau}$  with the rate-of-strain tensor  $\vec{\epsilon}$ ,

$$\Phi = \vec{\tau} : \vec{\epsilon} = 2\mu \vec{\epsilon} : \vec{\epsilon} + \lambda (\text{div } V)^2$$

where

$$\vec{\epsilon} = \frac{1}{2} [\text{grad } V + (\text{grad } V)']$$

$$\vec{\tau} = 2\mu \vec{\epsilon} + \lambda (\text{div } V) \vec{I}$$

In these relations,  $V$  is the fluid velocity,  $\mu$  and  $\lambda$  are the first and second coefficients of viscosity, and  $\vec{I}$  the unit tensor.

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We denote the mass fraction of species  $\alpha$  as  $y_\alpha$ . It is governed by a rate equation that can be written as

$$\rho \frac{Dy_\alpha}{Dt} = \rho \dot{\omega}_\alpha - \text{div} j_\alpha, \quad \alpha = 1, 2, \dots, N \quad (3)$$

where  $\dot{\omega}_\alpha$  is the rate of change of mass of species  $\alpha$ , per unit mass of mixture, due to chemical reactions. Thus,  $\dot{\omega}_\alpha$  is a sum over all of the reactions that alter  $y_\alpha$ .

For an open system, we have the thermodynamic relation

$$Tds = dh - \frac{dp}{\rho} - \sum_{\alpha=1}^N \bar{\mu}_\alpha dy_\alpha$$

where  $\bar{\mu}_\alpha$  is the chemical potential of species  $\alpha$ . With the substantial derivative replacing the ordinary derivative and with Eq. (3), we have

$$T \frac{Ds}{Dt} = \frac{Dh}{Dt} - \frac{1}{\rho} \frac{Dp}{Dt} - \sum_{\alpha=1}^N \bar{\mu}_\alpha \dot{\omega}_\alpha + \sum_{\alpha=1}^N \frac{\bar{\mu}_\alpha}{\rho} \text{div} j_\alpha$$

Equation (1) is combined with this relation to yield for a fluid particle,

$$\rho \frac{Ds}{Dt} = \frac{1}{T} \left[ \Phi - \rho \sum_{\alpha=1}^N \bar{\mu}_\alpha \dot{\omega}_\alpha - \text{div} q + \sum_{\alpha=1}^N \bar{\mu}_\alpha \text{div} j_\alpha \right] \quad (4)$$

where

$$q = q_E + q_R$$

A new energy flux vector  $q^*$  is defined as

$$q = q^* + \sum_{\alpha=1}^N \bar{\mu}_\alpha j_\alpha$$

Consequently, the two rightmost terms in Eq. (4) become

$$-\text{div} q + \sum_{\alpha=1}^N \bar{\mu}_\alpha \text{div} j_\alpha = -\text{div} q^* - \sum_{\alpha=1}^N j_\alpha \cdot \text{grad} \bar{\mu}_\alpha$$

With this relation and the identity

$$-\frac{\text{div} q^*}{T} \equiv -\text{div} \frac{q^*}{T} + q^* \cdot \text{grad} \frac{1}{T}$$

Eq. (4) becomes

$$\rho \frac{Ds}{Dt} = \rho \dot{s}_{\text{irr}} - \text{div} \frac{q^*}{T} \quad (5)$$

where

$$\dot{s}_{\text{irr}} = \frac{1}{\rho T} \left[ \Phi - \frac{1}{T} q^* \cdot \text{grad} T - \rho \sum_{\alpha=1}^N \bar{\mu}_\alpha \dot{\omega}_\alpha - \sum_{\alpha=1}^N j_\alpha \cdot \text{grad} \bar{\mu}_\alpha \right] \quad (6)$$

The rightmost term in Eq. (5) results in positive or negative entropy changes of a fluid particle by heat and mass transfer between the particle and its surroundings. Consequently,  $\dot{s}_{\text{irr}}$  represents the rate of entropy production per unit mass of the mixture by the various irreversible processes evident on the right side of Eq. (6).

In Ref. 3,  $\dot{s}_{\text{irr}}$  is written as  $d_s s/dt$ ; in Ref. 4, it is written as  $(ds/dt)_{\text{irr}}$ . We prefer our notation as conceptually clearer, e.g., there is no state variable for entropy production. The

second law now has the form

$$\dot{s}_{\text{irr}} = 0$$

for reversible processes and

$$\dot{s}_{\text{irr}} > 0$$

for irreversible processes.

For a mixture of thermally perfect gases,

$$\bar{\mu}_\alpha = h_\alpha - Ts_\alpha, \quad \alpha = 1, 2, \dots, N$$

where  $s_\alpha$  is the specific entropy of species  $\alpha$ . In this case, the energy flux vector simplifies to

$$\frac{q^*}{T} = -k \frac{\text{grad} T}{T} + \sum_{\alpha=1}^N s_\alpha j_\alpha + \frac{1}{T} q_R$$

The terms on the right represent, respectively, the entropy change caused by conductive heat transfer, mass transfer, and radiative heat transfer.

### General Coordinates

We can write Eq. (6) in nonsteady, general coordinates. The vector and tensor formulas are from Ref. 10 and are included in the Appendix for convenience.

The transformation from the Cartesian coordinates  $x_i$  to general coordinates  $\xi^j$  is given by

$$\xi^j = \xi^j(x_1, x_2, x_3, t), \quad j = 1, 2, 3$$

If we use the covariant or contravariant tensor components, the results will involve the components of the fundamental metric tensor  $g_{ij}$  (see Appendix). We avoid this complication by using the contravariant vector components and the mixed tensor components of the general system. Consequently, the scalar form of Eq. (6) can be written as

$$\rho \dot{s}_{\text{irr}} = \frac{1}{T} \left[ \Phi - \frac{(q^*)^j}{T} \frac{\partial T}{\partial \xi^j} - \rho \sum_{\alpha=1}^N \bar{\mu}_\alpha \dot{\omega}_\alpha - \sum_{\alpha=1}^N j_\alpha^j \frac{\partial \bar{\mu}_\alpha}{\partial \xi^j} \right] \quad (7)$$

where repeated coordinate indices are summed over. The viscous dissipation is

$$\Phi = \frac{\mu}{2} (V_{,i}^j + V_{,j}^i) (V_{,i}^j + V_{,j}^i) + \frac{\lambda}{j^2} \frac{\partial}{\partial \xi^m} (JV^m) \frac{\partial}{\partial \xi^n} (JV^n)$$

and  $J$  is the Jacobian of the transformation (see Appendix). Alternatively, Eq. (6) can be written using Cartesian components as

$$\rho \dot{s}_{\text{irr}} = \frac{1}{T} \left[ \Phi - \frac{q_j^*}{T} \frac{\partial T}{\partial \xi^k} \frac{\partial \xi^k}{\partial x_j} - \rho \sum_{\alpha=1}^N \bar{\mu}_\alpha \dot{\omega}_\alpha - \sum_{\alpha=1}^N (j_\alpha)_j \frac{\partial \bar{\mu}_\alpha}{\partial \xi^k} \frac{\partial \xi^k}{\partial x_j} \right]$$

where

$$\begin{aligned} \Phi = & \frac{\mu}{2} \left( \frac{\partial V_j}{\partial \xi^k} \frac{\partial \xi^k}{\partial x_i} + \frac{\partial V_i}{\partial \xi^k} \frac{\partial \xi^k}{\partial x_j} \right) \\ & \times \left( \frac{\partial V_j}{\partial \xi^k} \frac{\partial \xi^k}{\partial x_i} + \frac{\partial V_i}{\partial \xi^k} \frac{\partial \xi^k}{\partial x_j} \right) \\ & + \lambda \frac{\partial V_m}{\partial \xi^k} \frac{\partial V_n}{\partial \xi^p} \frac{\partial \xi^k}{\partial x_m} \frac{\partial \xi^p}{\partial x_n} \end{aligned}$$

The magnitude of  $\dot{s}_{irr}$  is a measure of the importance of the irreversible processes. It is given algebraically by Eq. (7) as a function of position and time. It may be evaluated for a particular fluid particle by utilizing Lagrangian coordinates. Since Eq. (7) is uncoupled from the equations of motion, it may be evaluated as an auxiliary equation during a numerical computation or after the computation is completed.

Once  $\dot{s}_{irr}$  is established, Eq. (5) can be utilized for the evaluation of  $s(\mathbf{x}, t)$ . In contrast to Eq. (7), a partial differential equation is to be solved for which an expression is needed for the substantial derivative. For any scalar  $F$ , the time derivative in general coordinates is related to the Cartesian time derivative by<sup>6</sup>

$$\left. \frac{\partial F}{\partial t} \right|_{x_i} = \left. \frac{\partial F}{\partial t} \right|_{\xi^j} + \frac{\partial F}{\partial \xi^k} \frac{\partial \xi^k}{\partial t} = \frac{\partial F}{\partial t} + \mathbf{w} \cdot \text{grad} F \quad (8)$$

where the velocity of the  $\xi^j$  coordinates is

$$\mathbf{w}^k = \frac{\partial \xi^k}{\partial t}$$

With Eq. (8), the substantial derivative in Eq. (5) becomes

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \text{grad}$$

where

$$\mathbf{u} = \mathbf{V} + \mathbf{w}$$

is a modified velocity that represents the sum of the fluid velocity and the velocity of the  $\xi^j$  coordinates.

### Appendix

The Cartesian base vectors are denoted as  $\hat{\mathbf{i}}_i$  and the covariant unitary base vectors of the general system are designated as  $\mathbf{e}_j$ . If  $\mathbf{A}$  is a vector and  $\vec{\sigma}$  and  $\vec{\pi}$  are tensors in the general system, it follows that

$$\mathbf{e}_i \cdot \mathbf{e}_j = g_{ij}, \quad \mathbf{e}_i \cdot \mathbf{e}^j = \delta_i^j$$

$$\mathbf{e}^j = g^{ij} \mathbf{e}_i, \quad \mathbf{e}_i = \frac{\partial x^j}{\partial \xi^i} \hat{\mathbf{i}}_j$$

$$J = \left| \frac{\partial \mathbf{x}_m}{\partial \xi^n} \right| = \mathbf{e}_i \cdot (\mathbf{e}_j \times \mathbf{e}_k) = g^{1/2}$$

$$\text{div} \mathbf{A} = \frac{1}{J} \frac{\partial}{\partial \xi^i} (J A^i)$$

$$\text{grad} \mathbf{A} = \mathbf{e}^j \frac{\partial}{\partial \xi^j} (A^i \mathbf{e}_i) = A^k_{,j} \mathbf{e}^j \mathbf{e}_k = A^k_{,j} g^{ij} \mathbf{e}_i \mathbf{e}_k$$

$$(\text{grad} \mathbf{A})^t = A^j_{,k} \mathbf{e}^j \mathbf{e}_k = A^j_{,k} g^{ij} \mathbf{e}_i \mathbf{e}_k$$

$$A^k_{,j} = \frac{\partial A^k}{\partial \xi^j} + A^i \{^k_{ij}\}$$

$$\{^k_{ij}\} = \frac{\partial \mathbf{e}_i}{\partial \xi^j} \cdot \mathbf{e}^k$$

$$\vec{\sigma} : \vec{\pi} = \sigma^i_j \pi^j_i$$

In the above,  $\delta^i_i$  is the Kronecker delta,  $J$  the Jacobian of the transformation,  $g$  the determinant of the fundamental metric tensor, and  $\{^k_{ij}\}$  the Christoffel symbol of the second kind.

### References

- <sup>1</sup>Salas, M. D. and Morgan, B. D., "Stability of Shock Waves Attached to Wedges and Cones," *AIAA Journal*, Vol. 21, Dec. 1983, pp. 1611-1617.
- <sup>2</sup>Powell, K. G., Murman, E. M., Perez, E. S., and Baron, J. R., "Total Pressure Loss in Vortical Solutions of the Conical Euler Equations," *AIAA Journal*, Vol. 25, March 1987, pp. 360-368.
- <sup>3</sup>Vincenti, W. G. and Kruger, C. H. Jr., *Introduction of Physical Gas Dynamics*, Wiley, New York, 1965.
- <sup>4</sup>Tolman, R. C. and Fine, P. C., "On the Irreversible Production of Entropy," *Reviews of Modern Physics*, Vol. 20, Jan. 1948, pp. 51-77.
- <sup>5</sup>Zhang, H., Camarero, R., and Kahawita, R., "Conservation Form of the Equations of Fluid Dynamics in General Nonsteady Coordinates," *AIAA Journal*, Vol. 23, Nov. 1985, pp. 1819-1820.
- <sup>6</sup>Warsi, Z. U. A., "Conservation Form of the Navier-Stokes Equations in General Nonsteady Coordinates," *AIAA Journal*, Vol. 19, Feb. 1981, pp. 240-242. (Note: the  $1/2$  coefficient in Eq. (10d) in this reference should be deleted.)
- <sup>7</sup>Emanuel, G., *Gasdynamics: Theory and Applications*, AIAA Education Series, 1986.
- <sup>8</sup>Arpaci, V. S., "Radiative Entropy Production," *AIAA Journal*, Vol. 24, Nov. 1986, pp. 1859-1860.
- <sup>9</sup>Bird, R. B., Stewart, W. E., and Lightfoot, E. N., *Transport Phenomena*, Wiley, New York, 1960, Sec. 18.4.
- <sup>10</sup>Reddy, J. N. and Rasmussen, M. L., *Advanced Engineering Analysis*, Wiley, New York, 1982.

## Moment Exerted on a Coning Projectile by a Spinning Liquid in a Spheroidal Cavity

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### Nomenclature

- $a$  = maximum radial distance of the liquid-filled container (for a cylinder, the radius; for a spheroid, the radial semiaxis)
- $c$  = one-half the maximum axial dimension of the liquid-filled container (for a cylinder, one-half the length; for a spheroid, the axial semiaxis)
- $f_s, f_c$  = fineness ratio,  $c/a$ , for a spheroid or cylinder, respectively
- $m_L$  = mass of the liquid in the completely filled container
- $Re$  = Reynolds number,  $a^2 \dot{\phi} \nu$
- $\epsilon$  = nondimensionalized damping
- $\nu$  = kinematic viscosity of the liquid
- $\tau$  = nondimensionalized frequency,  $\dot{\phi}_c / \dot{\phi}$
- $\phi_c$  = phase angle of the coning motion
- $\phi$  = spin rate with respect to inertial axes, assumed positive

### Introduction

THE prediction of the moment exerted by a spinning and coning projectile has been a problem of considerable interest to the Army for some time. For a spinning inviscid liquid in a cylindrical container, the linear liquid moment was first computed by Stewartson<sup>1</sup> by use of eigenfrequencies determined by the fineness ratio of the container. Wedemeyer<sup>2</sup>

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