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Entropy and the Second Law Fluid Flow and Heat Transfer Simulation

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A review of the diverse roles of entropy and the second law in computational thermo–fluid dynamics is presented. Entropy computations are related to numerical error, convergence criteria, time-step limitations, and other significant aspects of computational fluid flow and heat transfer. The importance of the second law as a tool for estimating error bounds and the overall scheme's robustness is described. As computational methods become more reliable and accurate, emerging applications involving the second law in the design of engineering thermal fluid systems are described. Sample numerical results are presented and discussed for a multitude of applications in compressible flows, as well as problems with phase change heat transfer. Advantages and disadvantages of different entropy-based methods are discussed, as well as areas of importance suggested for future research.

Nomenclature

c_p = specific heat, J/kg · K
E = total energy density, J/m^3
F = entropy flux
$\boldsymbol{\mathcal{F}}$ = flux column vector
I_S = entropy current
k = thermal conductivity, W/m · K
P = pressure, N/m^3
$\boldsymbol{Q}$ = vector of conserved variables
$\boldsymbol{q}$ = heat flux, W/m^2
R = gas constant per unit mass, m^2/s^2 · K
S = entropy density (volumetric), J/m^3 · K
$\dot{S}_{\text{gen}}$ = rate of entropy generation, W/m^3 · K
s = specific entropy, J/kg · K
T = absolute temperature, K
t = time, s
U = internal energy density, J/m^3
$\boldsymbol{v}$ = fluid velocity vector, m/s
x, y = Cartesian coordinates, m
γ = ratio of specific heats
Δ = increment or change of quantity
μ = dynamic viscosity, kg/m · s
ρ = mass density, kg/m^3
τ = viscous stress, N/m^2
Φ = viscous dissipation function, 1/s^2

Introduction

WE present a review of past advances in numerical analysis using the second law of thermodynamics. Entropy serves as a key parameter in achieving the theoretical limits of performance and quality in many engineering applications. Together with exergy, it can shed new light on various flow processes: from optimized flow configurations in an aircraft engine to highly ordered crystal structures (low entropy) in a turbine blade, as well as other applications. The many roles of entropy and the second law in computational fluid dynamics (CFD) will be reviewed.

Courant–Freidrichs–Lewy[1] (CFL) provided a major contribution to numerical analysis of thermofluid problems. The literature in this field often mentions that the CFL condition establishes a criterion in restricting the time step for linear differential equations to achieve numerical stability. However, it is not typically known that the CFL condition originally had nothing to do with numerical stability because that term was not phrased until the 1940s by a group associated with von Neumann.[2] The terminology remained, and today we understand the CFL condition as a necessary, and in some cases sufficient, condition for both numerical stability and convergence of linear equations. This paper will consider its link with the second law.

Subsequent advances included analytical techniques to determine the stability and convergence requirements for linear differential equations with constant coefficients and periodic boundary conditions.[3] The basic question of numerical stability deals with discretization error and roundoff error. Discretization errors are analogous to systematic errors that arise in experimental measurements, that is, they are a function of the method used. On the other hand, roundoff errors are analogous to the unpredictable and unavoidable errors that arise in the measurement process itself. Minimizing discretization errors requires very accurate approximations to terms that appear in the differential equations of interest. Roundoff errors often determine the success or failure of a method's stability.

The issue of numerical stability, in a strong sense, deals with the growth of the overall roundoff error.[4] In a weak sense, the growth of a single roundoff error is the question most frequently answered because it can be answered much more easily and practically.[5] Fourier error analysis answers the question of weak stability, and it is assumed that proof of weak stability, rigorous or heuristic, implies strong numerical stability. In the modern, practical use of CFD codes, we must often substitute heuristic arguments and rules of thumb to establish a restriction on the time step for explicit methods and time-accurate solutions. Often, numerical experimentation and trial and error are necessary to determine a method's stability bounds.

Typically neglected and often viewed as superfluous, the second law of thermodynamics remains an esoteric and mysterious subject.[6] Nevertheless, the physical basis and analogies inferred through the second law have significance in computational analysis of thermofluid systems. This paper outlines the reasons and mechanisms in which the second law is applied, that is, numerical stability,

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subgrid modeling, convergence criteria, numerical error, and so on. The computed entropy generation includes the effects of various responses of a thermofluid system on the variations of system properties. In this way, it can provide more relevant convergence and other indicators than criteria based on a single entity alone.

The logic intrinsic to the second law enforces positive (computed) entropy production rates, which previous authors have directly linked to stability criteria of numerical algorithms. Also, the necessary direction of change in physical processes, as outlined by the second law, is useful in subgrid modeling. In regards to nonlinear convergence, an entropy criterion for thermodynamic equilibrium can be used for phase sequencing during iterations of phase change computations. These examples and others are detailed in this paper, so that the relevance of the second law in numerical analysis is outlined. It is anticipated that these applications can demonstrate the promising potential of actively incorporating the second law into existing computer codes.

Second Law Formulation

Overview

The original background of thermodynamics, based on the science of heat, was intended to account for common experiences involving energy exchange by work and heat.[7] These experiences were formulated as the first law of thermodynamics, and together with entropy and the second law, have become the main foundations for the analysis of energy systems.[8,9] In conjunction with these physical systems, the concept of entropy has relevance in other applications, including computational analysis of these systems.

For example, perpetual motion machines violating the second law in conventional thermodynamic analysis have an analogy in computational studies, namely, numerical errors and nonphysical results. In this example, the physical basis in the second law offers a wider perspective of all types of numerical errors, rather than only selected types considered by a Taylor series analysis. Another example outlining the benefits of this physical basis involves error indicators, which typically become useful only in a limit as the element size approaches zero, with the mesh possessing certain features. Unlike these methods, the computed entropy generation can indicate when the results are nonphysical, regardless of mesh spacing or element shape. In these examples, the relevance of the second law arises through its unified, systematic, and physically based framework for the numerical analysis. Other examples outlining the transition and analogies from conventional thermodynamics to computational analysis, based on the second law, will be described.

The energy and entropy balances for a system may be written as

$$E_{\text{in}} - E_{\text{out}} = \Delta E \tag{1}$$

$$S_{\text{in}} - S_{\text{out}} + S_{\text{gen}} = \Delta S \tag{2}$$

where the subscripts in and out represent the transfer of that quantity with mass flow, work, or heat and gen refers to the generation or production of that quantity. S is a system property that represents entropy per unit volume, whereas S_{gen} is a nonproperty because it represents the generation of entropy. On a rate basis, the units of $\dot{S}_{\text{gen}}$ become watts per cubic meter degrees Kelvin.

In Eq. (2), terms on the right-hand side represent the change in the quantity. The first law, essentially, postulates the existence of a thermodynamic variable, total energy, which is a property of state. Energy can be exchanged between different forms, but not created or destroyed. The second law postulates the existence of another variable, total entropy, which is also a property of state by definition. Entropy and probability theory are closely related.[10] Unlike the first law, the entropy balance equation contains a nonnegative production term (established by experiment and elevated to an axiom on par with the first law).

The functional relation between entropy and the extensive thermodynamic variables can be interpreted from statistical considerations.[11–13] The real world, effectively, generates entropy according to the second law. These concepts apply universally to all known physical processes, and so it is evident that the second law in particular may provide something of value if we expect mathematical and numerical solutions of differential equations to reflect the physical world. Pioneers who applied a second law or entropy condition to numerical analysis realized this important discovery.[14,15] The key lies in developing a mathematical formula that indicates whether the second law is satisfied or not. Many ways exist to express this mathematical formula, just like there are many ways to state the second law. The essence of the second law postulates the existence of a functional S that is concave in the dependent variable for which we have a differential equation.[13] If we treat the entropy S as another state variable that can be transferred across the boundaries of a system, then the concavity property of entropy effectively translates into the balance equation (2) for the entropy that requires nonnegative entropy generation.[16]

On a rate basis, the entropy transport equation may be written as

$$\dot{S}_{\text{gen}} = \dot{S} + I_S \tag{3}$$

where $\dot{S}$ is the time rate of change of entropy contained by the system and I_S is the entropy current density due to either mass flow, or heating, or both. The second law stipulates that the rate of entropy generation must be nonnegative in all thermophysical processes, that is, $\dot{S}_{\text{gen}} \geq 0$.

Transport Form

The second law may be written in a transport form by writing the entropy balance equation of an open thermodynamic system as a partial differential equation as follows[17]:

$$\dot{S}_{\text{gen}} = \frac{\partial(\rho s)}{\partial t} + \nabla\cdot(\rho \mathbf{v} s) + \nabla\cdot\left(\frac{k\nabla T}{T}\right) \tag{4}$$

where s is the specific entropy density. For reversible processes described by the inviscid flow equations, entropy generation equals zero identically. Such processes entail zero heat transfer, without any form of irreversibilities, that is, mixing of two inviscid streams of different temperatures, or unrestrained expansion of such fluid. In this case, one can solve the governing equations without reference to the second law. However, in the presence of discontinuities such as shock waves, entropy generation must be nonnegative. For example, in the one-dimensional shock tube problem,[18] entropy generation is nonnegative. The maximum value of the specific entropy across the shock wave depends only on the upstream Mach number and the ratio of specific heats, just like the other thermodynamic variables in the Rankine–Hugoniot relations (see Refs. 19–21).

Positive Definite Form

An alternative positive definite form of the second law can be obtained as follows. Consider the one-dimensional form of the conservation of mass, balance of momentum, and conservation of energy equations,

$$\frac{\partial \boldsymbol{\mathcal{Q}}}{\partial t} + \frac{\partial \boldsymbol{\mathcal{F}}}{\partial x} + \frac{\partial \boldsymbol{\mathcal{F}}^v}{\partial x} = 0 \tag{5}$$

where $\boldsymbol{\mathcal{F}}$ and $\boldsymbol{\mathcal{F}}^v$ are the convective and viscous fluxes, respectively. The components of $\boldsymbol{\mathcal{Q}}$ are $\mathcal{Q}_1 = \rho$, $\mathcal{Q}_2 = \rho u$, and $\mathcal{Q}_3 = \rho e$. The flux vectors are given by

$$\boldsymbol{\mathcal{F}} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u e + p u \end{bmatrix}, \qquad \boldsymbol{\mathcal{F}}^v = \begin{bmatrix} 0 \\ -\tau \\ -u\tau + q \end{bmatrix} \tag{6}$$

The viscous effects associated with velocity gradients, which give the shear stress, as well as heat conduction contributing to the heat flux, are

$$\tau = \frac{4}{3}\mu\frac{\partial u}{\partial x}, \qquad q = -k\frac{\partial T}{\partial x} \tag{7}$$

These relations are based on the standard constitutive relations named after Stokes and Fourier, respectively (see Ref. 22).

The algebraic row vector containing the gradients of the entropy with respect to the conserved state variables is

$$S_{,Q} = [s + u^2/2\sigma^2 - \gamma/(\gamma - 1), -u/\sigma^2, 1/\sigma^2] \tag{8}$$

where $\sigma^2 = RT = (\gamma - 1)(2\mathcal{Q}_1\mathcal{Q}_3 - \mathcal{Q}_2^2)/2\mathcal{Q}_1^2$. In Eq. (8) the subscript notation with a comma refers to differentiation with respect to the indicated variable. When the scalar product is taken with Eq. (5), and the chain rule and compatibility condition[23] are used,

$$\frac{\partial S}{\partial t} + \frac{\partial F}{\partial x} + S_{,Q} \cdot \frac{\partial \boldsymbol{\mathcal{F}}^v}{\partial x} = 0 \tag{9}$$

On simplifying and using the constitutive relations for the stress tensor and heat flux, we get

$$\frac{\partial S}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial}{\partial x}\left(\frac{q}{T}\right) = \frac{4}{3}\frac{\mu}{T}\left(\frac{\partial u}{\partial x}\right)^2 + \frac{k}{T^2}\left(\frac{\partial T}{\partial x}\right)^2$$

Identifying the left-hand side as the entropy generation from Eq. (4) yields

$$\dot{S}_{\text{gen}} = \frac{4}{3}\frac{\mu}{T}\left(\frac{\partial u}{\partial x}\right)^2 + \frac{k}{T^2}\left(\frac{\partial T}{\partial x}\right)^2 \tag{10}$$

This result represents the one-dimensional positive definite form of the second law of thermodynamics. Equation (10) requires nonnegative entropy generation, which essentially restricts the coefficients of viscosity and conductivity to nonnegative values. The second law, when used in this capacity, effectively prescribes the constitutive relations allowed in physical theory. A derivation of this result from kinetic theory usually follows a more complex line of reasoning. The same expression can be constructed from the Navier–Stokes equations, requiring a more lengthy derivation utilizing the continuum extension of the Gibbs equation, which relates the entropy to the temperature, pressure, mass density, and internal energy. When Eq. (10) is generalized to multidimensions, the positive definite form of the second law becomes

$$\dot{S}_{\text{gen}} = \left(\frac{\mu\Phi}{T}\right) + \left[\frac{k(\nabla T \cdot \nabla T)}{T^2}\right] \tag{11}$$

where Φ refers to the viscous dissipation function.[17]

Entropy Equation of State

Inasmuch as entropy is not measured directly, but rather indirectly through other variables, an equation of state is required to evaluate entropy in terms of those variables. For incompressible substances, such as liquids or solids, the Gibbs equation yields a logarithmic variation of entropy S with temperature, that is,

$$S(T) = S_0 + \rho c_p \ln\left(\frac{T}{T_0}\right) \tag{12}$$

where the subscript 0 denotes a reference state. For multiphase mixtures, reference values of s_0, c_p, and T_0 are required in each phase to accommodate both sensible and latent heat components.[24]

For compressible flows, the entropy can be expressed by

$$S - S_0 = \rho R\left[\frac{1}{\gamma - 1}\ln\left(\frac{T}{T_0}\right) - \ln\left(\frac{\rho}{\rho_0}\right)\right] \tag{13}$$

$$S - S_0 = \rho c_v \ln\left[\frac{P/P_0}{(\rho/\rho_0)^\gamma}\right] \tag{14}$$

$$\frac{S - S_0}{\rho_0 R} = \frac{\rho}{\rho_0}\left[\frac{1}{\gamma - 1}\ln\left(\frac{T}{T_0}\right) - \ln\left(\frac{\rho}{\rho_0}\right)\right] \tag{15}$$

where Eq. (14) is derived from gasdynamics theory and Eq. (15) is nondimensionalized.

Boundary Conditions

In addition to the preceding forms of the second law and equations of state, boundary conditions are required to formulate fully the second law. Once the conservation variables are determined, their respective fluxes across the physical boundaries of the domain can be determined for closure of the entropy flows across those boundaries. Alternatively, the boundary entropy production rate can be calculated directly from Eq. (11). In this approach, only the spatial derivatives of temperature and velocity are computed along the boundaries for the boundary values of entropy production rate. In a numerical scheme, this approach would ensure positive definite results for the boundary entropy production rates.

Concavity Property

Two important mathematical properties of entropy have emerged as critically important for developing and applying the second law: concavity and compatibility. The first property requires a negative second derivative of entropy, that is,

$$S_{,QQ} < 0 \tag{16}$$

Equation (16) suggests that $S_{,QQ}$ must be a negative definite matrix, as a consequence of the second law, which requires that irreversible processes produce entropy. Entropy is bounded from above as it attains a maximum value at an equilibrium condition. This physical connection between the second law and concavity are clarified by the following example.

Consider a rigid-material body at some temperature T immersed in a thermal reservoir at a temperature of T_0, such as a hot rock inside a cool room. Suppose $T > T_0$, and we let the cooling process proceed from the initial time t to t_0 when the body reaches thermodynamic equilibrium with its surroundings. Based on an energy balance, the heat transfer from the object equals the difference between the object's initial internal energy U and its final internal energy U_0. Based on Eq. (2) with this heat outflow leading to S_{out}, the entropy generation associated with the cooling process becomes

$$S_{\text{gen}} = S_0 - S - (1/T_0)(U_0 - U) \tag{17}$$

To write the change of energy in terms of the change of temperature, we use the definition of specific heat ($C_V = \partial U/\partial T$) and a standard thermodynamic relation, that is,

$$\frac{C_V}{T} = \frac{\partial S}{\partial T} \tag{18}$$

so that Eq. (17) becomes

$$S_{\text{gen}} = S_0 - S - \left.\frac{\partial S}{\partial T}\right|_0 (T_0 - T) \tag{19}$$

Equation (19) indicates the concavity property of entropy as a function of T.

To clarify this meaning of Eq. (19), consider some arbitrary function $F = F(X)$ such that $F'' < 0$. The inequality indicates that F is a concave function of its argument.[25] Integrating by parts yields

$$-\int_{X_1}^{X_2} (X - X_1)F''(X)\,\mathrm{d} = F(X_2) - F(X_1) - F'(X_2)(X_2 - X_1) \tag{20}$$

Based on the concavity of F and the result on the right-hand side,

$$F(X_2) - F(X_1) - F'(X_2)(X_2 - X_1) \geq 0 \tag{21}$$

where the equality holds if and only if $X_2 = X_1$. Comparing Eq. (21) with Eq. (19) demonstrates that, for this case, nonnegative entropy generation (required by the second law) is equivalent to asserting the concavity property of entropy when $S = S(T)$. Similar examples can be constructed for other cases involving variations of entropy with more than one variable.

Compatibility Condition

The second important property of entropy is the following compatibility condition for reversible processes:

$$\boldsymbol{F}_{,Q} = S_{,Q}\boldsymbol{\mathcal{F}}_{,Q} \tag{22}$$

In Eq. (22), $\boldsymbol{F}_{,Q}$ refers to the entropy flux derivative matrix (second-order tensor). Also, $\boldsymbol{\mathcal{F}}_{,Q}$ is a third-order tensor because it describes a derivative of flux terms in three space directions with respect to the conservation variables. The compatibility condition represents a type of consistency condition between the fluxes of entropy and the conserved variables.

The importance of the compatibility condition is considered through an analysis of the following one-dimensional conservation law:

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0 \tag{23}$$

where $f(u)$ is the flux of u (dependent variable). The corresponding balance of entropy is represented by

$$\dot{S}_{\text{gen}} = \frac{\partial S}{\partial t} + \frac{\partial F}{\partial x} \tag{24}$$

In Eq. (24), F refers to the transfer of entropy with u.

Thermodynamically, $S = S(u)$, and let $S' = \mathrm{d}S/\mathrm{d}u$ refer to the first derivative of the entropy with respect to the variable u. Multiplying Eq. (23) by S', combining with Eq. (24), and using the chain rule of differential calculus gives

$$\dot{S}_{\text{gen}} = (F' - S'f')\frac{\partial u}{\partial x} \tag{25}$$

where $\partial F/\partial x = F'\partial u/\partial x$. Note that all terms on the right side can have positive or negative values. This opens the possibility for violation of the second law, which stipulates that $\dot{S}_{\text{gen}} \geq 0$.

To preclude such a condition, the second law, applied as a constitutive constraint, requires that

$$F' = S'f' \tag{26}$$

which represents the so-called compatibility condition. The literature sometimes introduces this condition as a separate axiom, for example, see Merriam,[26] whereas we have already shown that it actually follows from applying the second law principle directly. Thus, we have

$$\frac{\partial S}{\partial t} + \frac{\partial F}{\partial x} = 0 \tag{27}$$

by substitution and use of the chain rule once again. From Eq. (24), it follows that $\dot{S}_{\text{gen}} = 0$. This conclusion follows from the strictly conservative nature of Eq. (27). Theoretically, this condition holds as a limiting form of

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = \mu\frac{\partial^2 u}{\partial x^2} \tag{28}$$

which admits more general solutions and includes a dissipative transport mechanism.[27,28] This insight, although not new, leads to a novel approach in using the second law in its fundamental form for prescribing constitutive constraints for numerical calculations. More detailed discussions of concavity and compatibility conditions involving entropy are discussed by Camberos.[23]

Symmetric Hyperbolic Forms

Entropy and the second law can be used to transform the governing equations to exhibit certain desirable properties when discretizing these equations. The benefits of transforming the equations to symmetric hyperbolic forms have been investigated by Hughes et al.[29] and Harten et al.[30] Tadmor has used an entropy inequality to establish uniqueness and stability of a numerical scheme, after writing the governing equations in a special self-adjoint form.[31]

Exergy and Work Potential

Other benefits can be realized when constructing the entropy equations in terms of exergy, or work potential.[16,32] For example, the degradation of work potential due to irreversible losses can be expressed in terms of units of energy, which may have a more readily interpreted meaning. The earlier discussed concavity property of entropy translates into a corresponding mathematical property for exergy. In particular, the exergy must be a convex function of its thermodynamic variables.

Numerical Analysis

Second Law Discretization

When Eq. (4) is integrated over a discrete volume and time step,[33]

$$\dot{S}_{\text{gen}} \equiv \left(\frac{S_i^{n+1} - S_i^n}{\Delta t}\right)\Delta\mathcal{V} + \sum_{ip}\boldsymbol{F}_{ip}(\Delta\boldsymbol{\mathcal{S}}_{ip}) \geq 0 \tag{29}$$

where the subscripts i, ip and superscripts n, $n+1$ refer to nodal point, that is, center of control volume, integration point (at edges of the control volume), and time levels at the previous and current time steps, respectively. Also, $\Delta\mathcal{V}$ and $\Delta\mathcal{S}$ are the volume size and surface area enclosing the control volume, respectively. The discretization in Eq. (29) is based on the transport form of the second law in Eq. (4), whereas another representation can be obtained from the positive definite form of Eq. (11).

Once the solution variables from the conservation equations have been obtained, together with the entropy equation of state, the discrete entropy production rate can be determined from Eq. (29). Observe that a reconstruction step is required in Eq. (29) because the spatial distribution of the conservation variables must be determined from nodal values. Special caution must be exercised when calculating entropy in terms of those variables, so that the second law is not violated during that reconstruction step. A possible approach is to use piecewise constant values of the conservation variables, thereby assuming a type of quasi-equilibrium condition.[24]

Numerical Stability

The relevance of the second law in regards to numerical stability of fluid flow simulations has been documented by Merriam,[26] Dutt,[34] and others. For example, Merriam shows that a sufficient condition for numerical stability of a finite difference CFD model is a positive entropy production throughout the domain.[26] Numerical predictions that would otherwise become unstable may enhance entropy production through dissipation terms to ensure numerical stability. When the second law principle (nonnegative entropy generation) and the concept of entropy are expanded and developed, it can be shown that an alternative to linear stability analysis exists based on such concepts.

Because of the universality of the entropy concepts introduced, they apply to any of the common partial differential equations of thermal and fluid dynamics. These attempts seek to address the question of strong numerical stability by extending the modified equation technique pioneered by Warming and Hyett[4] and others. The modified equation for the balance of entropy provides a powerful yet simple method for gauging a numerical method's stability properties because numerical stability is directly related to the overall generation of entropy.[23] Additionally, the second law provides a way to gauge the local quality of the solution because spurious oscillations in the numerical solution can arise under conditions of entropy destruction.[26]

Uniqueness

Entropy and the second law have an important role in establishing the physically relevant and unique numerical solution of nonlinear equations.[14,27] Use of the second law in the context of numerical analysis and stability is not entirely new. In fact, soon after the concept of numerical stability was understood, work began in applying the second law, or something like it, to provide rational criteria for selecting the correct, that is, physically relevant solution to the partial differential equations of interest. Thus, by analogy, a pioneering use of the second law provided additional mathematical constraints that determined physically relevant solutions to the differential equations encountered. With such second law consideration, these equations often exhibit nonunique and discontinuous solutions.[15]

Artificial Dissipation

The second law offers a physically based and rigorous approach to artificial dissipation for numerical stabilitization.[35] The local entropy production rate provides a quantitative measure of the numerical dissipation added and the amount required for stable computations. It has been observed that an upwind bias to interpolation between grid points increases the entropy production in the adjacent elements.[26] Numerical schemes can be constructed to ensure that the second law is satisfied locally.[36] A limited diffusive flux (called smoothing) is added to stabilize a second-order finite difference scheme. In certain cases, satisfying the entropy constraint can be shown to be total variation diminishing (TVD).[36] Majda and Osher attempt to ensure compliance with the second law by modifying the numerical viscosity of numerical schemes.[37]

Nonphysical Results

Solutions of the conservation equations do not preclude results that may exhibit nonphysical behavior, such as undershoots or overshoots. In many instances, detailed grid refinements are too time consuming or expensive, or experimental data are not available, so that assessing the physical reliability of computed results is difficult. In those cases, the second law offers a physically based way of detecting the plausibility of such results.

The required amount of artificial dissipation, based on the second law, can be used to eliminate nonphysical results, including overshoots or undershoots. Consider the following results obtained by a control-volume-based finite element method.[33] In Figs. 1 and 2, a one-dimensional shock tube problem is shown.[18] Shock tubes are used for investigating various physical phenomena involving high-temperature gases in aerodynamics, transonic and supersonic flows, wave interactions, flame propagation, and chemical reaction kinetics. A diaphragm initially separates the tube into high- and low-pressure regions, but after it is removed, a shock wave propagates into the low-pressure section (right side) of the tube. In Fig. 2, the second law has been used to provide an entropy-based viscosity to reduce/eliminate the overshoot of predicted velocity at the shock wave position.[18] As detailed in Ref. 18, the entropy-based viscosity is a postprocessed calculation of numerical viscosity corresponding to the magnitude of entropy generation, as computed from the second law. It is based on a rearrangement of Eq. (11), in an effort to bring closer compliance of the CFD calculations with the second law. In this way, a predictive mechanism based on the second law is used to enhance the numerical stability and identify/remove nonphysical computed results.

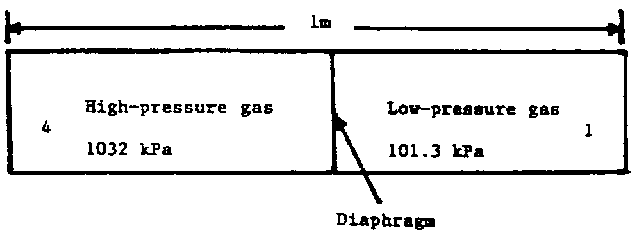

Fig. 1 Shock tube problem, where for air $R = 287$ J/kg · K, $c_p = 1004$ J/kg · K, $\gamma = 1.4$, and $T = 293$ K.

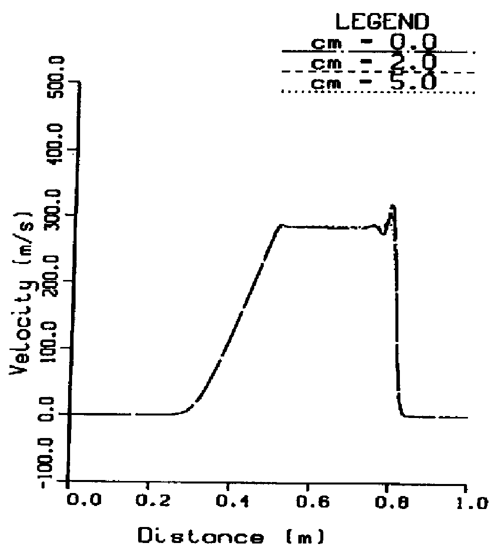

Fig. 2 Entropy corrected velocity.

Nonlinear Iterations

When the nonlinear conservation equations are solved, iterations are required between and within the equations until solution convergence is achieved. These iterations are continued until some acceptable reduction of the residuals has been obtained. The following residuals are defined, where the subscript i refers to node i and the superscripts n and $n+1$ refer to current and previous iteration values, respectively. Numerical iterations are continued until a representative solution residual falls below a specified tolerance. Examples of possible residuals are shown as follows.

Maximum mass density difference:

$$\mathrm{RES}_1 = \left|\rho_i^{n+1} - \rho_i^n\right|_{\max}$$

Mass density difference:

$$\mathrm{RES}_2 = \left\langle(\rho^{n+1} - \rho^n)_i^2\right\rangle^{\frac{1}{2}}$$

The rms pressure difference:

$$\mathrm{RES}_3 = \left\langle(p^{n+1} - p^n)_i^2\right\rangle^{\frac{1}{2}}$$

Average global entropy difference:

$$\mathrm{RES}_4 = |S(\boldsymbol{Q}^{n+1}) - S(\boldsymbol{Q}^n)|$$

It has been shown that fluid entropy serves as an effective generalized metric, which is indicative of residual error in iterations of the fluid flow equations.[38] Fluid entropy is relatively easy to calculate for gases, as well as incompressible substances. Also, entropy generation is a nonnegative quantity, which is important in certain numerical calculations. In such calculations, the magnitude of entropy is dependent on the selection of reference conditions for the entropy equation of state, that is, Eqs. (13–15).

Examples of such benefits of using entropy in nonlinear iterations are shown in Figs. 3 and 4 (Ref. 38). The explicit solutions in Figs. 3 and 4 were obtained based on the Euler equations with a variation on the Steger–Warming flux-vector splitting algorithm.[39]

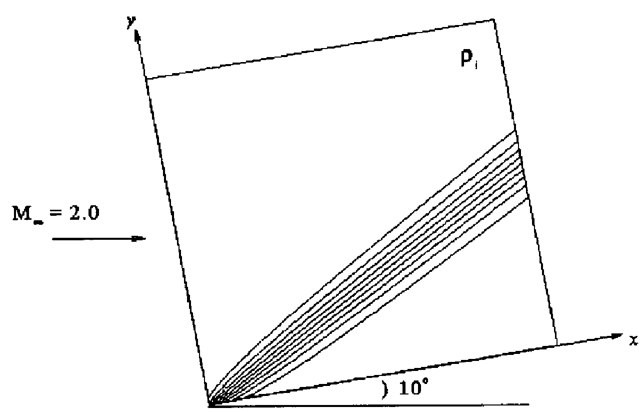

Fig. 3 Supersonic two-dimensional wedge flow.

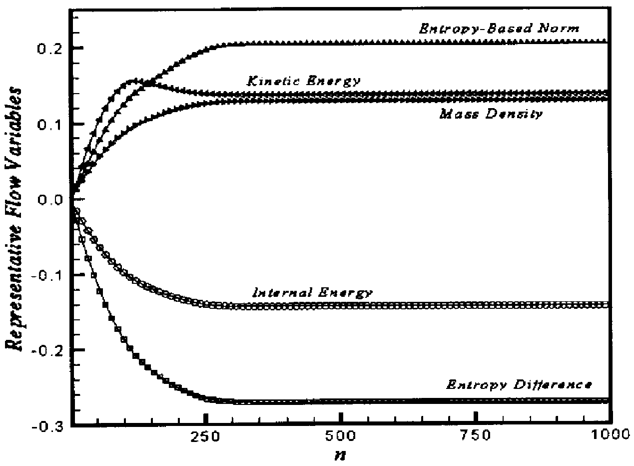

Fig. 4 Wedge flow results.

The upwind method includes flux-difference splitting.[40] An explicit solution of a supersonic two-dimensional wedge flow is shown in Figs. 3 (density contours) and 4 (iteration history for flow variables). The oblique shock wave is oriented at the correct location as predicted by theoretical gasdynamics. (Note smearing of shock wave due to the explicit, first-order scheme.) Solution convergence is achieved after about 300 iterations. Because the entropy-based norm is functionally dependent on all state variables, it is shown to provide a reliable criterion for establishing convergence of the nonlinear iterations.[38] In Fig. 4 and upcoming results, the entropy-based norm is defined as the average entropy difference over the computational domain (weighted by the local grid cell spacing), as indicated by the earlier defined RES_4 and further detailed in Ref. 38. Similarly, the other variables illustrated, such as mass density, kinetic energy, and so on, are defined analogously with respect to the average difference of that variable over the domain. For example, the mass density curve is based on the earlier defined RES_2.

When iterations of nonlinear equations involving phase change heat transfer are performed, the second law can be used in guiding these iterations.[24] In phase change problems, a tentative phase distribution is required before the solution of the governing equations. If the computed solution yields a different phase distribution than that tentative distribution, then further iterations are required until convergence between these distributions is achieved. The second law can be effectively used in this iterative process. In particular, the tentative phase within a control volume should yield a positive entropy production rate. If the second law is violated, then an entropy-based correction may be applied to accelerate the iterative process.[24,41]

Convergence Criteria

A numerical solution of a thermofluid problem is said to be converged when further calculations at the given time step will have little or no effect on the flowfield representation. Such convergence is determined by numerical criteria, such as a selected residual decreasing below a specified tolerance. An entropy-based residual, RES_4, was defined earlier, thereby introducing the relevance of the second law in convergence criteria. Fluid entropy, $S = S(\boldsymbol{Q})$, is functionally dependent on all state variables, thereby making it an effective choice as a convergence indicator. Also, entropy has a physically relevant significance embodied by the second law, which gives convergence studies a unique physical perspective. Previous studies have shown the effectiveness of entropy-based residuals in assessing various convergence characteristics of a numerical method.[38]

An important question involves how to minimize the number of iterations without compromising the quality of a numerical solution. It may be sufficient to measure the residual error by monitoring the difference in the slope as entropy changes with each time step. This would have to be done once the residual has dropped three or four orders of magnitude from its initial value, to make sure that the iteration curve for the representative variable (entropy) has "flattened out" enough.

Figures 5–8 illustrate some applications in gasdynamics that use entropy as a parameter in reaching solution convergence. A supersonic two-dimensional Prandtl–Meyer centered expansion (explicit) is illustrated in Figs. 5 (Ref. 38) and 6. Contours of constant Mach number are shown in Fig. 5 for supersonic flow over a convex corner. This flow configuration leads to a centered Prandtl–Meyer expansion fan. The orientation and location of the predicted expansion fan agree closely with the analytic solution of this problem. Figure 6 shows the iteration history for the flow variables in this problem. Although kinetic energy appears convergent after 100 iterations, the iteration histories of other variables flatten out after about 250 iterations. This result indicates that a representative flow variable that takes into account all state variables, that is, entropy difference or norm, should be used in the convergence criterion. Otherwise, the iterations may be prematurely terminated. Entropy possesses the important benefit of physical significance embodied by the second law of thermodynamics.

Supersonic two-dimensional blunt-body flow is shown in Figs. 7 (Ref. 38) and 8. This problem is a good example of a problem

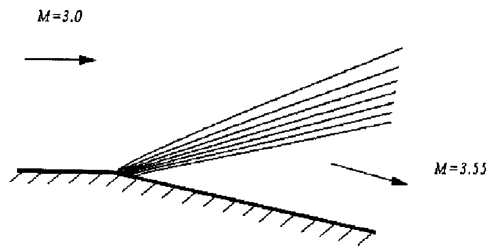

Fig. 5 Prandtl–Meyer two-dimensional expansion.

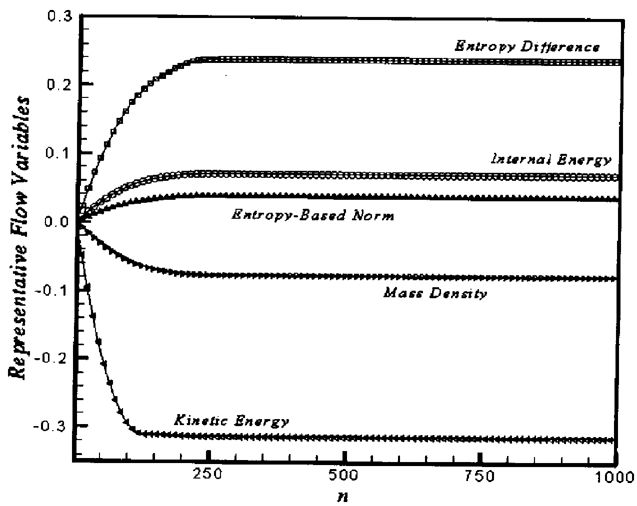

Fig. 6 Computed Prandtl–Meyer flow results.

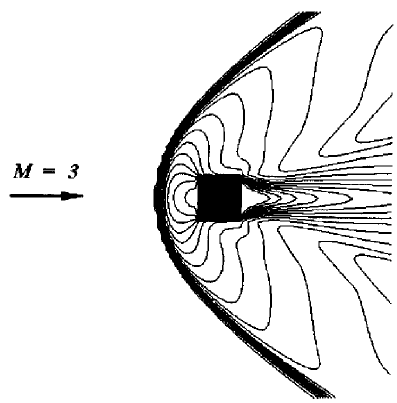

Fig. 7 Supersonic blunt-body flow.

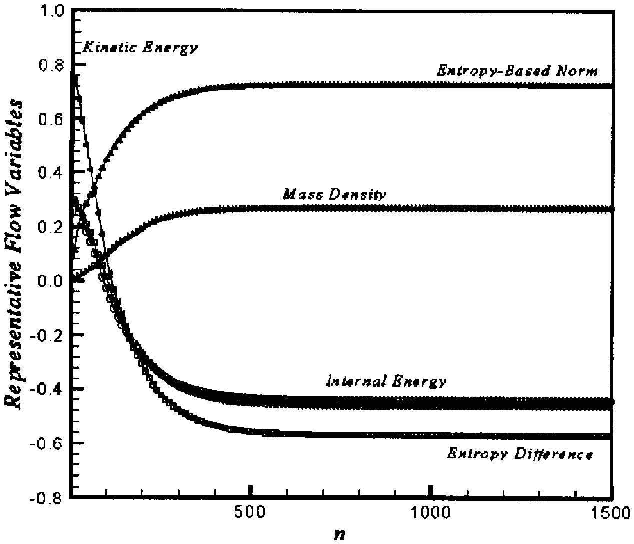

Fig. 8 Blunt-body flow results.

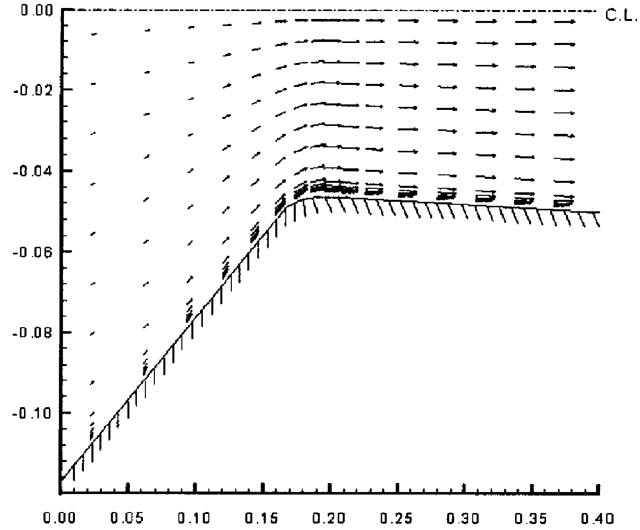

Fig. 9 Nozzle two-dimensional flow.

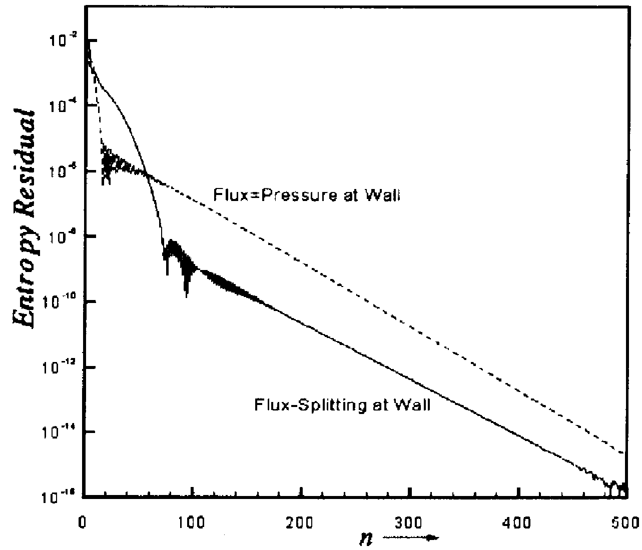

Fig. 10 Error metrics.

exhibiting the formation of a bowed shock wave. Because the numerical results of Mach number contours in Fig. 7 were obtained with a first-order, explicit scheme, the bowed shock is thick, but located approximately at the correct position as predicted by theoretical gasdynamics. Similar entropy results of iteration history in Fig. 8 give further evidence of the robustness and applicability of an entropy-based norm for two-dimensional problems involving curved shock waves.

Numerical Error

Unlike conventional error indicators based on Taylor series methods, the second law offers a physical basis from which CFD error analysis can be studied. In typical error indicators, it is often difficult or impractical to evaluate higher-order derivatives therein because those derivatives may be unbounded. On the other hand, the inequality of the second law may be used to assess systematically the errors without such higher-order derivatives. Harten et al.[42] use certain entropy conditions as a way of reducing overshoot and undershoot errors in compressible flow computations. Because it can place bounds on the solution norm,[43] the second law has relevance in outlining the bounds of numerical errors. Other studies have demonstrated that such errors are accumulated when certain second law conditions are violated.[44]

In certain cases, there exist direct relationships between numerical error and the apparent error in entropy production.[45] The difference between entropy production rates, computed based on their positive definite and transport forms, can be used as a more general error indicator for coarse grids. Also, a weighted entropy residual can serve as an effective error indicator.[46] Because of its physical basis in the second law, these entropy-based error indicators can encompass more types of numerical errors, including both overall and individual parts of the formulation, rather than only certain types of errors. Unlike other conventional finite element error indicators limited to restricted classes of problems,[47] the second law offers a promising physically based alternative to better understand and predict numerical errors.

An example using an entropy-based error metric is shown in Figs. 9 and 10. The implicit solution for the nozzle problem was obtained by a Gauss–Seidel line relaxation technique for the thin-layer Navier–Stokes equations. The results from converging–diverging two-dimensional nozzle flow are summarized in Figs. 9 and 10 (Ref. 38). The lower portion of the nozzle is shown with the nozzle centerline corresponding to the upper portion of Fig. 9. The inlet conditions are subsonic and the velocity vectors are shown in Fig. 9. In Fig. 10, the following two methods are used for imposing the wall boundary condition: 1) specified normal flux term equal to pressure at the wall and 2) flux-splitting technique using the layer of cells adjacent to the wall to create a layer of "ghost cells" with the normal velocity component reflected. In both methods, the residual error metric based on the entropy difference indicates solution convergence at about 50–70 iterations.

Subgrid Modeling

When applied locally, the second law has relevance in subgrid modeling because its inequality imposes certain constraints on the variables discretized. If such constraints are violated locally, then numerical errors can be traced back to the corresponding local approximations made. In this way, a link between subgrid modeling and the second law can be established. For example, Merriam shows that an upwind bias to interpolation between grid points increases the entropy production in the adjacent elements.[26]

Consider another specific example involving convective upwinding. In Boltzmann-type schemes, convective transport is based on phase–space trajectories of individual "particles." In modified Boltzmann schemes, that is, those of Deshpande,[48] Reitz,[49] and Pullin,[50] a series of error functions are computed (based on normal probability densities) to derive the difference equations. Other examples of convective upwinding include the exponential differencing scheme and skew upwind differencing scheme. In numerical upwinding, an approximation of the local transported quantity, that is, velocity at the edge of a control volume, is required in terms of surrounding nodal values. These local upwinding approximations should not be averse to the requirements of the second law.

In terms of the conserved variables $\mathcal{Q}$ and associated flux terms $\mathcal{F}$, it can be shown that their subgrid evaluation can be written in terms of entropy as follows[33]:

$$\dot{S}_{\text{gen}} = S_{,\mathcal{Q}}(\mathcal{Q}_{,t} + \mathcal{F}_{,x}) + \tfrac{1}{2}S_{,tt}\Delta t \geq 0 \qquad (30)$$

The numerical entropy production of each individual contribution should be high enough to prevent a net negative sum, that is, prevent a violation of the second law. Otherwise, it is anticipated that the resulting computational error may lead to weak convergence or unstable results. Individual discrete approximations can be assembled together into Eq. (30). Then, the second law can be enforced locally through proper subgrid modeling. In this way, errors associated with individual components of the overall model, such as numerical upwinding, can be reduced through compliance with the second law.

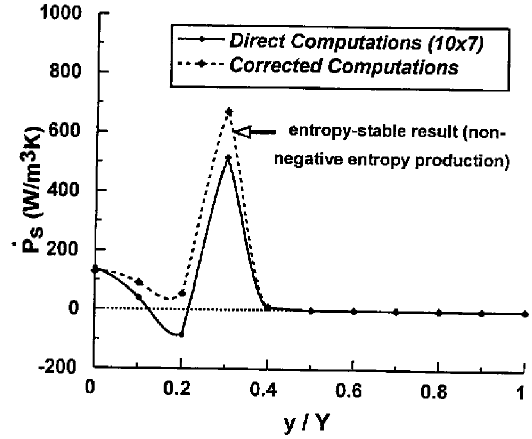

Fig. 13 Entropy production.

Predictive–Corrective Measures

The second law can provide a useful basis for predictive–corrective measures in numerical calculations. An example involving phase change heat transfer in an enclosure is shown in Figs. 11 and 12 (Ref. 51). In that analysis, the magnitude of computed negative entropy production is used in a corrective manner to improve the solution accuracy. Discretization errors, due to inadequate spatial or temporal differencing, may lead to such negative values. If the second law is violated locally, then a quantitative indication of the diffusivity required (denoted by k_s) to correct the solution may be expressed in terms of the negative entropy production rate (absolute value), based on Eqs. (4) and (11), that is,

$$k_s \approx |\dot{P}_s| \left[\frac{T^2}{\nabla T \cdot \nabla T} + \frac{T}{\Phi}\left(\frac{c_p}{Pr}\right) \right] \qquad (31)$$

When this entropy-based diffusivity is used, the corrected solution can achieve closer compliance with the second law, thereby leading to more stable computations with reduced numerical error.

Sample results from this type of predictive–corrective algorithm are shown in Fig. 12. In Fig. 12, an entropy-based conductivity has been used to improve the numerical accuracy of the predicted interface position, while improving the overall numerical stability. (Note that Fo refers to Fourier modulus, or dimensionaless time.) This improvement is quantified with respect to computed positive entropy production in accordance with the second law (Fig. 13). Other examples of entropy-based corrections of numerical heat transfer are cited in the literature, for example, Nellis and Smith.[52]

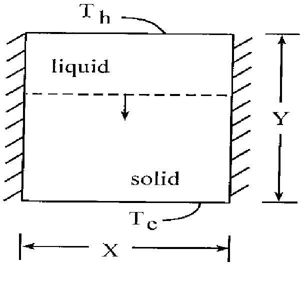

Fig. 11 Phase change schematic.

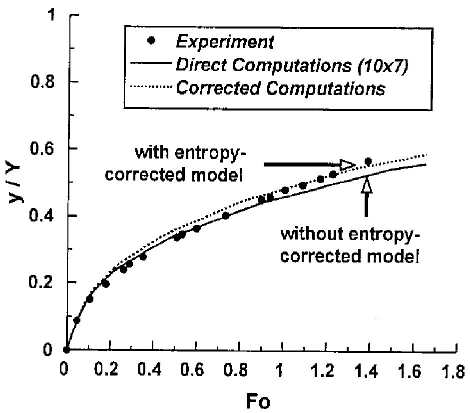

Fig. 12 Interface position.

Time Step Limitations

Time step restrictions for stable time advance, as well as the second law, both involve inequalities. Use of the second law in properly selecting the time step size has been reported previously.[44,53] Numerical approximations, as already discussed, generally do not result in zero entropy generation, even for the simulation of adiabatic, inviscid fluid flow. In the context of explicit time advance, consider the following strategy for securing numerical stability in view of time step selection and the second law:

1) Write the numerical formula for the conservation law as an explicit update equation for approximating the exact solution.

2) Write the approximation error $\mathcal{L}_\Delta$ according to $\mathcal{L}_\Delta \equiv [u(t+\Delta t, x) - u_j^{n+1}]/\Delta t$. Then, expand all terms in a Taylor's series, equating the result, up to the truncation error, to zero.

3) Derive the expression for the entropy generation by multiplying the error from step 2 by S' and use the compatibility property to simplify.

4) Analyze the leading error terms to enforce nonnegative entropy generation, by analogy with the second law. Then, an inequality involving the time step may be derived.

Other conditions, such as monotonic conditions,[54] are sufficient but not necessary conditions for numerical stability. For linear equations, the CFL conditions and results from a second law analysis satisfy the monotonic requirement in some cases. However, for nonlinear equations, it has been shown that the CFL condition can lead to over- or underpermissive time step restrictions.[53] The logic of an entropy-based approach is deeply rooted in the physical/mathematical theory that gives its universality and power, the second law of thermodynamics. It is this universality that can be exploited to provide a physically based way of establishing the proper time step size.

As an example of this approach, consider a one-dimensional problem combined with the second law to identify a nonlinear time step constraint for stable computations. The discrete operator for the scalar transport equation, $\mathcal{L}^d(\mathcal{Q})$, is written in terms of the analytic (differential) operator, $\mathcal{L}^a(\mathcal{Q})$, and higher-order terms arising from the Taylor series expansion (see Ref. 44), that is,

$$\mathcal{L}^d(\mathcal{Q}) = \mathcal{L}^a(\mathcal{Q}) + \tfrac{1}{2}\rho u^0(u^0\Delta t - \Delta x)\mathcal{Q}_{,xx} \qquad (32)$$

where u^0 refers to a characteristic, or lagged, velocity for linearization of the nonlinear convection term. Also, Δt and Δx refer to the time step and grid spacing, respectively. In Eq. (32), the discrete operator depends on the second-order spatial derivative of the scalar $\mathcal{Q}$ and higher-order terms (neglected).

Then, through pre-multiplication by an entropy derivative, S_Q, the preceding result can be transformed into an expression for the entropy production rate, that is,

$$\dot{S}_{\text{gen}} = -\tfrac{1}{2}\rho u^0(\Delta x - u^0 \Delta t) S_{,QQ}(\boldsymbol{Q}_{,x})^2 \geq 0 \qquad (33)$$

The second law requires a positive entropy production rate, so that

$$u^0 \Delta t / \Delta x \leq 1 \rightarrow \text{CFL condition} \qquad (34)$$

As a result, the well-known CFL condition[1] for numerical stability follows from the second law under the conditions outlined for this example problem. Thus, the second law can provide a physical basis and guidance for the selection of appropriate time steps for stable computations.

Inverse Methods

In the earlier described direct problems, the solutions of the fluid flow and heat transfer equations give the consequences, that is, velocity or temperature distribution, of a given cause, that is, boundary condition. On the other hand, an inverse analysis attempts to find the unknown causes of known or desired consequences.[55] Inverse problems can be ill posed in the sense that small perturbations in observed measurements may lead to large changes in the solution. As a result, special techniques such as entropy-based techniques may be adopted to stabilize the computations arising in inverse solutions.

A measured or desired characteristic of a problem, such as interface motion in phase change problems, can be controlled through a boundary condition (such as boundary temperature). In this case, a sensitivity coefficient is often used in inverse problems to describe the effect of a change in the controlling variable (boundary temperature) on the controlled variable (interface position). However, as the interface moves farther away from the boundary, the sensitivity coefficient decreases such that it becomes more difficult to control the interface motion from the external boundary. As a result, numerical oscillations are often coincident with resulting instabilities. It has been shown that the second law can provide a physically based stability mechanism.[56] In particular, if negative entropy production is computed in the vicinity of numerical oscillations, then a corrective mechanism (based on this negative value) may be applied before the next time step. In this way, an entropy corrected sensitivity coefficient may provide a robust and effective alternative to conventional stabilizing techniques, such as future time stepping, that is, using estimated future coefficient values.

Consider an example where the boundary temperature at the left wall is used to control the motion, position, and shape (all specified) of the advancing phase interface in Fig. 14 (Ref. 56). Although the predicted decrease of the wall temperatures in Figs. 15 and 16 agree well with analytical solutions at early periods of time, some discrepancy arises after long periods of time. Numerical instability arises from reduced sensitivity coefficients in the inverse solution once the interface moves sufficiently far from the controlling boundary [Fig. 15 (Ref. 56)]. The oscillations are reduced/eliminated, and the algorithm is stabilized by an entropy-based correction in view of the second law.

Further details regarding the problem parameters, boundary and other conditions for problems reported in this section are outlined in Refs. 18, 38, 51, and 57. These references also include documentation involving verification and validation of the computed results, as well as other detailed information in regards to quantified accuracy of the results.

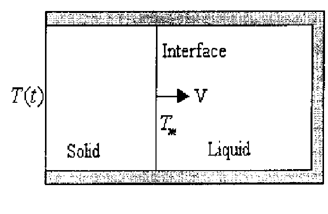

Fig. 14 Inverse problem.

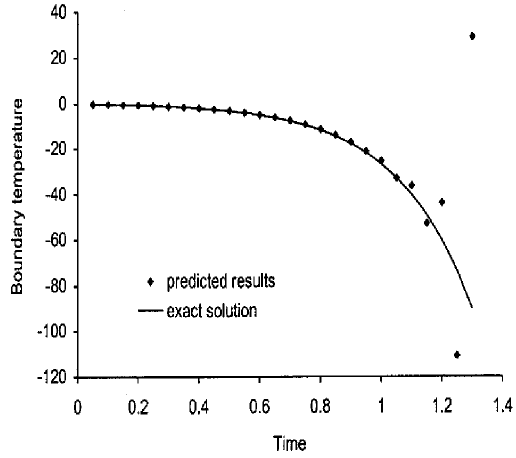

Fig. 15 Without entropy correction.

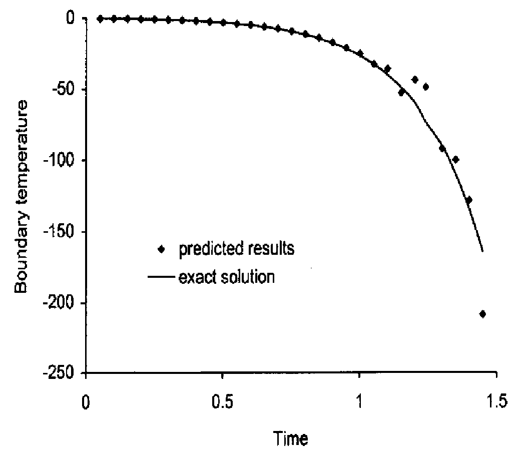

Fig. 16 With entropy correction.

Applications

Flow and Phase Change Phenomena

Compressible Flows

It appears that the earliest applications of the second law to CFD predictions were made in the context of compressible flows.[28,57] Many of the techniques and sample results presented in preceding sections were developed for compressible flows. Other applications are described by Cox and Argrow,[58] as well as Borth and Argrow.[59] In those and other studies, compressible flow solutions in complex flowfields are analyzed in view of the second law. Compressible flows represent an important type of CFD problem where the importance of the second law has been well established.

Incompressible Flows

Although less documented than compressible flows, the second law has been applied to some incompressible flow CFD studies. For example, Drost and White[60] use a numerical method to predict the local rate of entropy production due to a fluid jet impinging on a heated wall. These calculations are used to optimize the design of an impinging jet heat exchanger. The optimum jet Reynolds number, which minimizes the entropy generation in the jet, is determined. Other incompressible flow studies include work by Cheng et al.,[61] whereby entropy production is used in the analysis of mixed convection in a vertical channel with transverse fin arrays.

Phase Change Heat Transfer

Predictive models of phase change heat transfer are widely used in a variety of practical applications, such as materials processing, that is, casting solidification, extrusion, and injection molding; manufacturing, that is, welding and rapid prototyping; deicing of aircraft and other structures; and thermal energy storage. In phase change applications, another mechanism of entropy production, namely, the entropy of phase transformation, is encountered.[62] As with earlier applications, entropy can serve as an effective parameter for better understanding of various physical processes during phase change. For example, interface properties and roughness are determined from the entropy change during solid–liquid phase transition. In solidification problems, dendritic arms often grow in a direction corresponding to the maximum thermal irreversibility because it is aligned with the heat flow direction, that is, direction of local temperature gradient. Other examples, such as thermal recalescence, are linked to the entropy change and production during phase transition.[63]

Certain modifications of earlier results are required when considering phase change problems. For solid–liquid systems, the entropy generation at the phase interface (subscript i) becomes[17]

$$S_{\text{gen},i} = \frac{\rho_s}{\rho_l}\left(\Delta S_f - \frac{\Delta E_f}{T}\right) + \frac{k_l}{\rho_l V_i}\frac{\mathrm{d}T}{\mathrm{d}n}\bigg|_l \left(\frac{1}{T_l} - \frac{1}{T_s}\right) \geq 0 \quad (35)$$

where $\Delta S_f = s_l - s_s$ is the entropy of fusion (approximately equal to the heat of fusion divided by the phase change temperature). The subscripts l, s, and f refer to liquid, solid and fusion, respectively. In this type of two-phase mixture, the entropy generation includes effects such as viscous dissipation due to shear action along a dendrite arm, as it moves a discrete distance over a specified time interval. Entropy generation in other multiphase systems is documented in Ref. 17.

Turbulence

Turbulence in a flowfield usually enhances the production of entropy. Numerical predictions of entropy production in a turbulent boundary-layer flow were presented by Moore and Moore.[64] A finite volume method for predicting the mean viscous dissipation and entropy production in turbulent flows, based on the time-averaged turbulence equations, was described by Kramer-Bevan.[65] The method is applied to turbulent flows in diffusers to identify flow losses and to attempt to develop better diffuser designs. Also, Herard uses entropy characterizations to develop stable algorithms for turbulence modeling.[66] A more robust compressible flow solver is considered, while using a splitting technique in agreement with entropy inequalities. Overall, a relative lack of documented work indicates the need for further work regarding turbulent entropy transport modeling.

Systems and Processes

From engineering thermodynamics to economics, biology, information/coding theory, and other disciplines, the various forms and applications of entropy are widespread. In the applied sciences, the second law offers a unified way to strive toward meeting the upper limits of technology performance. In certain ways, the existence of entropy can be considered independently of the second law.[67] Entropy and the second law have significance in many technologies of importance, including aerospace systems, heat exchangers, and others.

Aerospace Systems

Minimizing entropy production is equivalent to minimizing exergy destruction. In that regard, exergy can be used as a effective basis for developing a unified framework for aircraft system design, from the overall system level down to each component.[68,69] Incorporating the second law in this way precludes the possibility of nonphysical design scenarios, and it expands the horizon of possible improvements. It can provide a more complete system integration that connects all results in a design involving a common metric, namely, entropy production (or exergy destruction). Furthermore, it can better evaluate tradeoffs between dissimilar technologies within this unified system context. For example, the U.S. Air Force Research Laboratory has investigated exergy-based ways of developing a unified framework for the design, analysis, and optimization of next-generation aerospace vehicles.[70] In these methods, the second law is used as a fundamental design constraint to complement traditional methods based on the first law.

Heat Exchangers

In the design of heat exchangers, a typical goal involves increasing the rates of heat transfer, without excessively increasing the pressure drop throughout the system. Ratts and Brown[71] use entropy-generation minimization (EGM) to improve the system efficiency of a cascading refrigeration cycle, involving heat exchangers. Many thermal techniques, such as fins and baffles, are effective in enhancing the rate of heat transfer, but at the expense of excessive pressure losses. This tradeoff can be effectively expressed through a desired minimization of total entropy production. Thus, combining CFD and entropy generation predictions in applications involving heat exchangers is a worthy undertaking. Examples of such studies are given in Refs. 72–76.

Turbomachinery

When the local sources of losses are identified through flow irreversibilities, better turbomachinery designs can be developed. For example, Sciubba discusses the benefits of calculating entropy locally, thereby leading to improvements in the design of axial turbines.[77] Turbomachinery predictions typically involve several aspects of flow classifications discussed earlier, such as compressibility, turbulence, and possibly phase change.

Materials Processing

Entropy production has important consequences in various materials processing technologies. For example, the microstructures and morphological stability of a solidified phase interface are dependent on the molecular disorder at the interface, that is, entropy transport. The extent of entropy change during thermal processing of materials affects the molecular disorder and properties of the solidified material.[78]

Entropy predictions can give deep insight into various fundamental material processes. Consider an example involving iron oxide processing, whereby the oxide can have a square symmetry of atoms in the iron surface where the oxide grows. Entropy and atomic symmetry are closely related, and so microscale entropy predictions can give important clues about what causes corrosion in this material. Furthermore, consider materials used in electronics applications for semiconductor technologies. For instance, concentric hexagonal pits in cadmium sulfide (a widely used semiconductor) have a high crystal symmetry. Dislocation defects can largely degrade the electrical properties of this semiconductor, that is, increase/decrease conductivity by 1000–100,000 times. In this context, dislocation defects could be reduced through minimal entropy production during material formation.

Microelectronics Cooling

Another example application of significance is effective cooling of microelectronic assemblies. Predicted entropy production can be used to find the minimum power input to achieve convective cooling of an electronic package.[79] This minimization of entropy production is carried out with respect to the heat transfer contact area and coolant flow rate. It has been documented that the upper limits of faster and more compact computing circuits are closely linked to the second law.[80] For each base unit of entropy produced in a microelectronic assembly, this production corresponds to an amount of heat that could have been removed through appropriate cooling, but was not removed due to the system irreversibilities.

Optimization of Thermofluid Systems

A broader goal of incorporating entropy predictions into CFD solvers is to use these predictions for system level optimization purposes. Local EGM with numerical methods provides extra flexibility, in terms of geometrical configuration, in addition to analytical methods.[81,82] For example, applications involving entropy production with natural convection in cavities are presented by Baytas.[83] Darcy's law and the Boussinesq approximation are used, whereas the second law is discretized with a finite difference method. The predicted entropy generation gives useful information for the selection of a suitable angle of inclination of the cavity. This represents a physical example of how entropy predictions can complement standard CFD solvers. In other recent advances, the global optimization of irreversibility, or global maximization of flow access, has shown that a complete flow architecture can be derived from this constructal principle.[84] Also, it has been shown that the optimal configuration is situated where the imperfections (such as entropy generated by flow resistance) are distributed evenly through a heterogeneous flow system. Many other advances and applications are expected to become evident in future research.

Conclusions

A review of the diverse roles of entropy and the second law in computational thermofluids has been presented. It has been shown that the second law is closely related to discretization error, numerical stability, and other characteristics of numerical models. Assessing the reliability and performance of a computational model typically requires validation through comparisons with available experimental data. However, in many applications, experimental testing is too time consuming or expensive. In the absence of proper benchmark data, the second law provides an important tool for establishing error bounds. Areas of recommended future research include extensions of CFD entropy predictions to more complex physical processes, such as multiphase, reacting, and turbulent flows. Also, ensuring that computational methods obey the second law is expected to provide stronger links to numerical stability, well-established error bounds, and robustness.

Acknowledgment

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