

ENTROPY PRODUCTION MODELING IN CFD OF TURBULENT COMBUSTION FLOW

Ivar S. Ertesvåg*, Jostein Kolbu†
Department of Energy and Process Engineering
Norwegian University of Science and Technology
NO-7491 Trondheim, Norway

Abstract

A model for predicting the detailed field of entropy production by computational fluid dynamics (CFD) of turbulent flows with combustion is developed. The model is based on the widely used Eddy Dissipation Concept for turbulent combustion (EDC) by Magnussen and co-workers. It can be applied with an infinitely-fast-chemistry assumption or in conjunction with a detailed chemical mechanism (e.g. GRI Mech). The model is tested for a simple laboratory flame. The results are good when compared with results from a conventional box-model (overall) entropy-balance analysis.

Keywords: Turbulent combustion, EDC, CFD, entropy production, irreversibility

INTRODUCTION

For several decades, the methods of 2nd-law or exergy analysis of thermal and chemical systems have been developed and utilized. These methods are primarily flowsheeting approaches, where energy and exergy balances are put up for a number of interconnected subsystems or components (e.g. compressors, combustors, heat exchangers). Then the entropy production or the irreversibility (a.k.a. “lost work”) of each component can be computed.

In parallel, methods for computing detailed flow-fields without and with chemical reactions have been developed (known as computational fluid dynamics, CFD). In the context of turbulent combustion, Magnussen’s EDC has become a standard model for technological applications. These methods provide detailed fields of velocity, temperature and concentrations of species throughout combustors or other devices.

For accurate optimization, a more detailed knowledge of the entropy production may be desired. The CFD approach can be extended to provide a detailed field of the entropy production as well. The basic formulation for this is known from several textbooks. For laminar flows, these equations can be solved numerically, see e.g. [9]. However, as most

flows are turbulent, a model for entropy production is required, along with the models for turbulent transport, mixing, and combustion. One of the few attempts (the only?) is presented in [8], where combustion modeling was based on a prescribed-pdf method. In the present study, entropy modeling is based on the EDC [2–4, 6].

BASIC THEORY

Transport equations

The notation, terminology and basic assumptions are primarily those customarily used in fluid-mechanics and combustion literature (e.g. [2, 7, 10]). In some instances this differs from the irreversible-thermodynamics literature. The exposition follows an Eulerian and barycentric description, and continuity is assumed. The flow and scalar fields of reacting flows can be described by the following partial differential equations, often known as transport equations.

Momentum:

$$\underbrace{\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j)}_{\rho D u_i / D t} = \frac{\partial}{\partial x_j}(-p \delta_{ij} + \tau_{ij}) + \rho f_i. \quad (1)$$

Here, ρ is density, u_i Cartesian velocity components,

*ivar.s.ertesvag@ntnu.no

†jostein.kolbu@ntnu.no

p pressure, τ_{ij} is the viscous stress tensor, f_i body-force acceleration, and δ_{ij} is the Kronecker tensor.

Mass of species:

$$\rho \frac{DY_k}{Dt} = \frac{\partial}{\partial x_j} (-j_{k,j}) + R_k. \quad (2)$$

Here, Y_k is the species mass fraction, $j_{k,j}$ the mass flux, and R_k the volumetric reaction rate. When this equation is summed for all species, the continuity equation is obtained:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = \frac{D\rho}{Dt} + \rho \frac{\partial u_j}{\partial x_j} = 0. \quad (3)$$

Energy:

$$\rho \frac{De}{Dt} = \frac{\partial}{\partial x_j} \left(-q_j - \sum_k h_k j_{k,j} \right) - p \frac{\partial u_j}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + Q \quad (4)$$

Here, e is the specific internal energy of the mixture, q_j the heat flux, h_k the specific enthalpy, and Q the volumetric energy production, either by internal sources (heating) or by radiation. The second last term is the dissipation term, in the following denoted Φ . This equation can readily be rewritten into an equation for the enthalpy, $h = e + p/\rho$.

Flux relations

The preceding equations includes terms for molecular fluxes. For most combustion cases, and indeed turbulent combustion cases, the following models are appropriate. For Newtonian fluids, the viscous stress tensor is expressed

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_l}{\partial x_l} \delta_{ij}. \quad (5)$$

Mass diffusion is modeled by Fick's law,

$$-j_{k,j} = \rho \mathcal{D}_k \frac{\partial Y_k}{\partial x_j}, \quad (6)$$

and heat transfer by Fourier's law,

$$-q_j = \lambda \frac{\partial T}{\partial x_j}. \quad (7)$$

Here, the dynamic viscosity μ , the thermal conductivity, λ , and the specific heat capacity, c_p , are for the mixture, whereas the diffusion coefficient, \mathcal{D}_k , is for the individual species.

Entropy

Later on, we will make use of the fact that the chemical potential (here used on a mass basis) for ideal gases is equal to the specific Gibbs function:

$\mu_k = g_k = h_k - Ts_k$. With material derivatives, the classical Gibbs' equation can be expressed

$$T\rho \frac{Ds}{Dt} = \rho \frac{De}{Dt} - \frac{p}{\rho} \frac{D\rho}{Dt} - \rho \sum_k \mu_k \frac{DY_k}{Dt}. \quad (8)$$

From this and the energy and mass balances, an entropy equation can be developed on the form

$$\begin{aligned} \rho \frac{Ds}{Dt} = & \frac{\partial}{\partial x_j} \left(-\frac{q_j}{T} - \sum_k s_k j_{k,j} \right) \\ & + \left(-\frac{q_j}{T^2} \right) \frac{\partial T}{\partial x_j} + \frac{1}{T} \sum_k (-j_{k,j}) \left(\frac{\partial \mu_k}{\partial x_j} \right)_T \\ & + \frac{Q}{T} + \frac{\Phi}{T} - \frac{1}{T} \sum_k \mu_k R_k. \end{aligned} \quad (9)$$

TURBULENCE MODELING

Averaging

For turbulent reacting flows, it is convenient to include the density in the averaged quantities. This is known as mass-weighted Reynolds average or Favre average [2, 7]. The quantities such as velocity, specific enthalpy, species mass fraction, and temperature are decomposed into mean and fluctuating values as $\phi = \tilde{\phi} + \phi''$, where ϕ is a general variable. The mass-weighted mean value is defined

$$\tilde{\phi} = \frac{\overline{\rho\phi}}{\bar{\rho}}. \quad (10)$$

A consequence of this definition is that $\overline{\rho\phi''} = 0$, whereas in general, $\overline{\phi''} \neq 0$. The overbar shows average (statistical expectation). If the density does not fluctuate, or does not correlate with the other quantity, the Favre average is equivalent to the Reynolds average.

Continuity

The mass-weighted Reynolds-averaged (Favre-averaged) continuity equation is

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j) = 0. \quad (11)$$

Momentum and turbulence transport

The mass-weighted Reynolds average (Favre average) momentum equation can be written

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(\bar{\tau}_{ij} - \overline{\rho u_i'' u_j''}) + \bar{\rho} f_i. \quad (12)$$

This is a derivation from Eq. (1). The new quantities appearing in this equation, $\overline{\rho u_i'' u_j''}$, represent convective transport of mean momentum by the action of turbulent motion. Their effect is similar to the (viscous) stresses, and they are known as Reynolds or turbulence stresses. From these, the turbulence energy is defined $\bar{\rho}\tilde{k} = \frac{1}{2}\overline{\rho u_i'' u_i''}$. A simple and frequently used model for the Reynolds stresses is the turbulence-viscosity model:

$$-\overline{\rho u_i'' u_j''} = \mu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \left(\bar{\rho}\tilde{k} + \mu_t \frac{\partial \tilde{u}_l}{\partial x_l} \right) \delta_{ij}. \quad (13)$$

This model is an analogy to Eq. (5). However, the turbulence viscosity, μ_t , is not a material property but a quantity characteristic of the flow. It can be regarded as a product of a turbulence length scale and a turbulent velocity scale. These scales can be expressed from lengths and velocities of the flow situation. However, a more general approach is to solve these scales from transport equations. The by far most popular model, which will be used here, is the k - ε model. Then the turbulence viscosity is modeled

$$\mu_t = \bar{\rho} C_\mu \frac{\tilde{k}^2}{\tilde{\varepsilon}} \quad (14)$$

Similar quantities, representing turbulence transport of scalars, will appear in mean-scalar transport equations in the following. When a general scalar is denoted ϕ , the Reynolds or turbulence fluxes are modeled

$$-\overline{\rho \phi'' u_j''} = \Gamma_{\phi,t} \frac{\partial \tilde{\phi}}{\partial x_j} = \frac{\mu_t}{\sigma_\phi} \frac{\partial \tilde{\phi}}{\partial x_j}. \quad (15)$$

This is known as the general gradient model. The turbulence Prandtl/Schmidt numbers, σ_ϕ , have to be specified in the model. The mean molecular diffusive flux may also be modeled by the same formalism or by more exact expressions of that term.

It should be noted that models solving transport equations for the Reynolds stresses are also an re-

alistic option for turbulent combusting flows. However, these aspects of turbulence modeling are beyond the scope of this study.

Turbulence energy and dissipation rate

The modeled transport equation for turbulence energy can be written

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{k}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{k}\tilde{u}_j) = P^k + D^k + \Pi^k - \bar{\rho}\tilde{\varepsilon}. \quad (16)$$

In this equation, the production term,

$$P^k = -\overline{\rho u_i'' u_j''} \frac{\partial \tilde{u}_i}{\partial x_j}, \quad (17)$$

is closed as the Reynolds stresses already are modeled. The model expressions for the remaining terms vary according to the chosen model. The diffusion term is usually modeled by a molecular term and a turbulence term according to the general-gradient model,

$$D^k = \frac{\partial}{\partial x_j} \left(\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial \tilde{k}}{\partial x_j} \right). \quad (18)$$

The pressure term, Π^k , is very often neglected, as a generic and fully accepted model is still to be developed. Finally, the dissipation rate of turbulence energy,

$$\bar{\rho}\tilde{\varepsilon} = -\overline{\tau_{ij} \frac{\partial u_i''}{\partial x_j}}, \quad (19)$$

is solved from a separate transport equation. The terms as shown here follows the "standard" k - ε model for high-Reynolds number flows [5].

The dissipation-rate equation can be written

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{\varepsilon}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{\varepsilon}\tilde{u}_j) = D^\varepsilon + S^\varepsilon, \quad (20)$$

where the diffusion term is modeled analogously to Eq. (18) in the turbulence energy equation,

$$D^\varepsilon = \frac{\partial}{\partial x_j} \left(\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \tilde{\varepsilon}}{\partial x_j} \right), \quad (21)$$

and the source term is modeled as a balance between production and destruction:

$$S^\varepsilon = \frac{\tilde{\varepsilon}}{\tilde{k}} \left(C_1 P^k - C_2 \bar{\rho}\tilde{\varepsilon} \right). \quad (22)$$

Mass of species

The transport equation for mean mass fraction is

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_k) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{Y}_k\tilde{u}_j) = \frac{\partial}{\partial x_j} \left(-\overline{j_{k,j}} - \overline{\rho Y_k'' u_j''} \right) + \overline{R_k}. \quad (23)$$

The diffusive molecular and turbulence fluxes of species mass are often modeled according to the general gradient model, corresponding to Eq. (15) or Eq. (18) above. Moreover, the reaction term (species production term) has to be modeled, see below.

Energy

The energy equation, Eq. (4), can be rewritten to an enthalpy equation. The averaged version of this equation is

$$\begin{aligned} \frac{\partial}{\partial t}(\bar{\rho}\tilde{h}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{h}\tilde{u}_j) &= \frac{\partial \bar{p}}{\partial t} + \tilde{u}_j \frac{\partial \bar{p}}{\partial x_j} + u_j'' \frac{\partial p}{\partial x_j} \\ &+ \frac{\partial}{\partial x_j} \left(-\bar{q}_j - \sum_k \overline{h_k j_{k,j}} - \overline{\rho h'' u_j''} \right) + \bar{\Phi} + \bar{Q} \end{aligned} \quad (24)$$

In this equation, the third term at the right-hand side is equivalent to the pressure term Π^k in Eq. (16), and has to be modeled (often neglected).

The treatment of the diffusive fourth term depends both on the approximations for the heat and the molecular flux and on the numerical approach. However, the third part, the turbulence diffusion of enthalpy, is modeled according to the general gradient model, Eq. (15).

Combustion modeling

The Eddy Dissipation Concept for turbulent combustion (EDC) [2–4, 6] can be used to model the interaction between turbulence and combustion. A cascade model is used to link the fine turbulence structures (where reactions are assumed to occur) to the mean flow and large-scale turbulence (that is described by turbulence models). The fine structures are modeled as a reactor, Fig. 1. The reaction rate is obtained from a mass balance for each species.

When a fast-chemistry assumption (*i.e.* “mixed is burnt”) is applied, the average reaction rate in Eq. (23) is modeled

$$\bar{R}_{\text{fu}} = -\frac{\bar{\rho}\gamma^* \dot{m}^* \chi}{1 - \gamma^* \chi} \tilde{Y}_{\text{min}}, \quad (25)$$

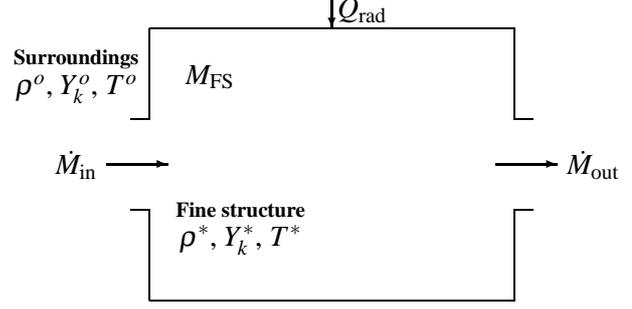


Figure 1: Schematic fine structure reactor of EDC

where

$$\tilde{Y}_{\text{min}} = \min \left(\tilde{Y}_{\text{fu}}, \frac{1}{r} \tilde{Y}_{\text{ox}} \right). \quad (26)$$

Here, r is the stoichiometric oxidizer (*i.e.* air or oxygen) requirement on a mass basis for the specific fuel, and subscripts “fu” and “ox” denote fuel and oxidizer, respectively. The quantities γ^* and \dot{m}^* are the mass fraction of turbulence fine structures and its mass exchange with the surrounding fluid, respectively (cf. Fig. 1). These are related to the turbulence-cascade model of the EDC [2, 3] and are expressed as functions of the turbulence energy \tilde{k} and its dissipation rate $\tilde{\epsilon}$. The chemical reactions are assumed to occur in the fine structures, *i.e.*, the small turbulence scales. The mass exchange is the reciprocal of the fine-structure residence time, $\tau^* = 1/\dot{m}^*$, which is proportional to the Kolmogorov time scale. The quantity χ is the fraction of fine structure that is reacting, and is a function of the concentrations of fuel, oxidizer, and product. The implementation of chemical kinetics is described by [4]. Then the reaction rate for a chemical species is expressed

$$\bar{R}_k = -\frac{\bar{\rho}\gamma^* \dot{m}^*}{(\gamma^*)^{1/3}} (Y_k^o - Y_k^*). \quad (27)$$

Here, Y_k^o and Y_k^* are the mass fraction of species k entering into and leaving the fine-structure reactor, respectively. The reacting turbulence fine structures are regarded as a perfectly stirred reactor, and the species mass balances of the reactor is solved with the use of data from a chemical-kinetics mechanism (*e.g.* GRI-Mech).

The model in Eq. (27) is obtained from a species mass balance for the reactor (Fig. 1), while Eq. (25) is the special case for fast chemistry. An energy balance for the reactor provide a model for the reactor

and mean temperatures. Similarly, we will use an entropy balance to model the entropy production.

Mean Entropy Equation

Above, the transport equation for entropy was expressed from the equations for species mass, continuity, and energy, by using Gibbs' relation. However, for the mean quantities, there exist no simple relation corresponding to the Gibbs relation or Eq. (8.)

The equation for the average of the entropy, can be written as the mean of Eq. (9),

$$\begin{aligned} \frac{\partial}{\partial t}(\bar{\rho}\bar{s}) + \frac{\partial}{\partial x_j}(\bar{\rho}\bar{s}\tilde{u}_j) \\ = \frac{\partial}{\partial x_j} \left(\overline{-\frac{q_j}{T} - \sum_k s_k j_{k,j} - \rho s'' u_j''} \right) \\ + \overline{\left(-\frac{q_j}{T^2}\right) \frac{\partial T}{\partial x_j}} + \overline{\sum_k \left(-\frac{j_{k,j}}{T}\right) \left(\frac{\partial \mu_k}{\partial x_j}\right)_T} \\ + \overline{\left(\frac{Q}{T}\right)} + \overline{\left(\frac{\Phi}{T}\right)} - \overline{\left(\frac{1}{T} \sum_k \mu_k R_k\right)} \end{aligned} \quad (28)$$

The five last terms are the mean entropy production. It should be noted that the average of the products and ratios are not readily rewritten into terms containing products of mean values. This means that models for transport and production of mean entropy have to be developed.

As an example of the required modeling, the viscous-dissipation term can be inspected: The dissipation term of the entropy equation can be split in a mean-flow term and a turbulence term,

$$\overline{\left(\frac{\Phi}{T}\right)} = \overline{\left(\frac{\tau_{ij}}{T}\right) \frac{\partial \tilde{u}_i}{\partial x_j}} + \overline{\frac{\tau_{ij}}{T} \frac{\partial u_i''}{\partial x_j}} = \overline{\left(\frac{\tau_{ij}}{T}\right) \frac{\partial \tilde{u}_i}{\partial x_j}} + \overline{\left(\frac{\rho \varepsilon}{T}\right)}. \quad (29)$$

Notice here that ε denotes the non-averaged dissipation rate of turbulence energy, cf. Eq. (19).

Provided that, but only then, the correlations between temperature and the other quantities are weak, the mean temperature can be left outside. For the viscous term, this is a reasonable assumption. However, for the other terms, the assumption would imply that the fluctuations of temperature and species mass fractions were small – which is certainly not the case in turbulent combustion.

ENTROPY MODELING WITH THE EDDY DISSIPATION CONCEPT

Overall approach

Turbulent motion may be regarded as eddies of sizes ranging from the external dimensions of the flow down to the smallest scales where the eddies are disrupted by viscous forces. This can be depicted as an energy cascade [3]. Combustion takes place at all scales, but mainly in the smallest scales. There, the gradients, and hence, the molecular fluxes, are the largest. Similarly, entropy is produced at all scales but mainly in the smallest eddies of turbulence.

When modeling the entropy production with the EDC, the approach will be to split the production into a large-scale (i.e. mean-flow and large-scale turbulence) contribution and a fine-structure contribution.

$$P^{\bar{s}} = P_{\text{LS}}^{\bar{s}} + P_{\text{FS}}^{\bar{s}} \quad (30)$$

The large-scale contributions to entropy production are modeled by using the mean values in the production terms:

$$P_{\text{LS}}^{\bar{s}} = \frac{\bar{\tau}_{ij}}{\bar{T}} \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\lambda}{\bar{T}^2} \left(\frac{\partial \bar{T}}{\partial x_j}\right)^2 + \sum_k \frac{\mathcal{R}_u \bar{\rho} \mathcal{D}_k}{M_k \bar{Y}_k} \left(\frac{\partial \bar{Y}_k}{\partial x_j}\right)^2. \quad (31)$$

Here, \mathcal{R}_u is the universal gas constant, and M_k is the molar mass. The radiation term is neglected in this study. In the EDC, the reactions are assumed to take place in the fine structures, and hence, there are no large-scale contributions from reactions.

Turbulence fine-structure entropy modeling

In the EDC, a mass-weighted (Favre) average (cf. Eq. 10) is expressed [2, 6] as

$$\tilde{\phi} = \gamma^* \chi \phi^* + (1 - \gamma^* \chi) \phi^o. \quad (32)$$

The general variable ϕ can represent the entropy production, σ . Thus, $\bar{\rho} \tilde{\sigma} = \bar{\rho} \bar{\sigma}$ is the mean of the sum of entropy-production terms of Eq. (9), and σ^* and σ^o are the entropy production rates on a mass basis of the reactor and its surroundings, respectively. Here, in conjunction with Eq (30), the contribution of fine-structures to mean entropy production will be modeled by

$$P_{\text{FS}}^{\bar{s}} = \bar{\rho} \tilde{\sigma}_{\text{FS}} = \bar{\rho} (\gamma^* \chi \sigma^* + (1 - \gamma^* \chi) \sigma^o). \quad (33)$$

This formulation is based on the assumption in EDC that all reactions take place in the reactor. Furthermore, the major part of localized heat and mass exchange due to reactions also take place in the reactor or its vicinity. After exiting the reactor, the products are mixed with the surroundings.

Similar to the mass and energy balances [2], an entropy balance for the reactor can be put up to determine the reactor entropy production,

$$\sigma_1^* = \dot{m}^* \sum_k (Y_k^* s_k^* - Y_k^o s_k^o) - \frac{Q_{\text{rad}}}{\rho^* T^*} \quad (34)$$

Here, the notation of the EDC is followed: The superscripts $*$ and o refer to properties of the reactor and the surroundings of the reactor, respectively. \dot{m}^* is the mass inflow rate to the reactor divided by the mass of the reactor. Its reciprocal is the residence time of the reactor. The last term is entropy transferred by radiation inflow, cf. Fig. 1. In this study, radiation term is neglected. However, when a radiation model is implemented with the combustion model (for energy exchange), it can readily be implemented in the entropy production model as well. The expression above does not include the post-reaction mixing. This can be modeled

$$\sigma_2^* = \dot{m}^* \sum_k (Y_k^* (s_k^* - \tilde{s}_k)) \quad (35)$$

for the mass exiting from the fine-structure reactor. Here, \tilde{s}_k denotes the entropy of the species based on mean composition, pressure and temperature. The two contributions should be added; $\sigma^* = \sigma_1^* + \sigma_2^*$. At this stage, the last term of Eq. (33), σ^o , is left for future considerations.

The model in Eqs. (33)-(35) is decoupled from the specific formulation of the terms in Eq. (9). The idea of this model is that reactants enter the reactor with properties of the surroundings, whereas products leave the reactor with properties of the reactor. The model can be used both with the "fast chemistry" assumption, and with a detailed mechanism for chemical kinetics. When EDC is implemented in a code, the quantities Y_k^* , Y_k^o , T^* , and T^o are already computed. Then, the mole fractions X_k^* and X_k^o and the partial pressures p_k^* and p_k^o can readily be calculated. Eventually, the only task remaining is to determine the specific entropies

$$s_k^* = s_k(T^*, p_k^*) \quad \text{and} \quad s_k^o = s_k(T^o, p_k^o). \quad (36)$$

For readers familiar with the EDC, it can be mentioned that a simpler expression involving \tilde{Y}_{min} (cf. Eq. 25) is not obtainable for the model in Eq. (34).

The investigations of [1] indicate that the reactions as such only give a minor contribution to entropy production, compared to the associated mass and energy exchange. Basically, the model in Eqs. (33)-(35) should be a model including all the localized (small-scale) entropy-producing processes in the turbulent combusting flow. That is, all processes (e.g. local mass transfer) that affects the field of temperature and partial pressures. Even though the individual processes are not specified, when their effects are seen in the temperature and composition fields, they are also included in the entropy-production model.

PREDICTIONS

For exemplary calculations, the model was applied to a jet flame. The fuel is a 1:1 mixture of H_2 and N_2 , and the fuel jet diameter, bulk velocity, and Reynolds number are 8 mm, 34.8 m/s, and 10000, respectively. The jet is situated in a air coflow with diameter 400 mm, and velocity 0.2 m/s. Both flows have temperature 300 K. This is case "H3" in the database of the International Workshop on Measurement and Simulation of Turbulent Non-premixed Flames. The predictions were made using the general-purpose CFD code Spider, which is based on finite volumes and non-orthogonal curvilinear computational mesh. In this case, a 2-dimensional rectangular mesh with axial symmetry was used. The turbulence model was the standard k - ϵ model, except for the round-jet modification of the constant $C_2 = 1.83$ (Eq. 22) and turbulence Prandtl and Schmidt numbers of 0.5. Buoyancy was included in the momentum equation. Combustion was modeled with the EDC and fast-chemistry assumption (Eqs. 25–26). Thermophysical data, including enthalpy and entropy, were obtained from the Chemkin Library.

The inlet boundary was specified as fixed values. For the jet flow, these were approximated to calculations of a fully developed pipe flow. The outlet was a parallel flow, and at the outer boundary zero radial transport was assumed.

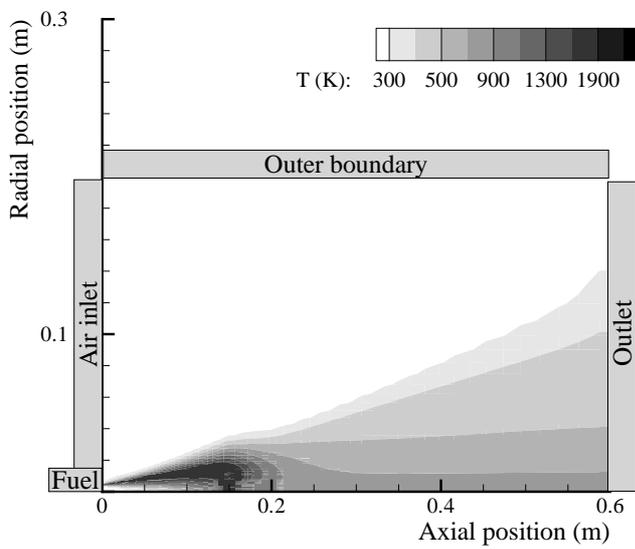


Figure 2: Geometry and computed mean temperature field of the flame

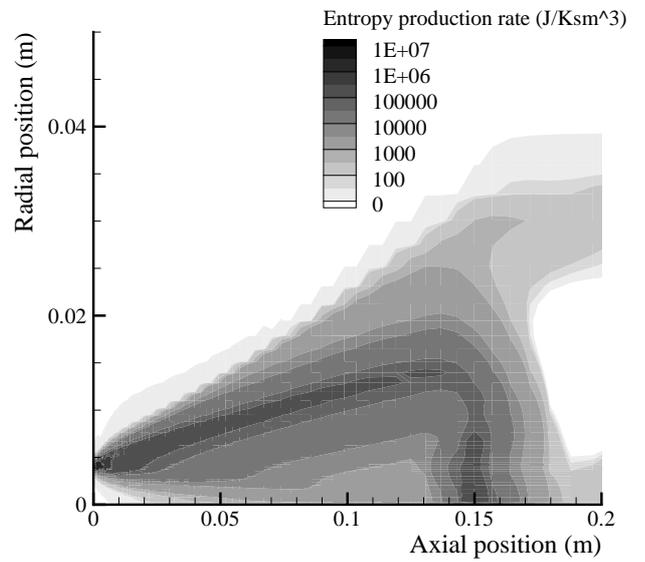


Figure 4: Zoomed excerpt from Fig. 3

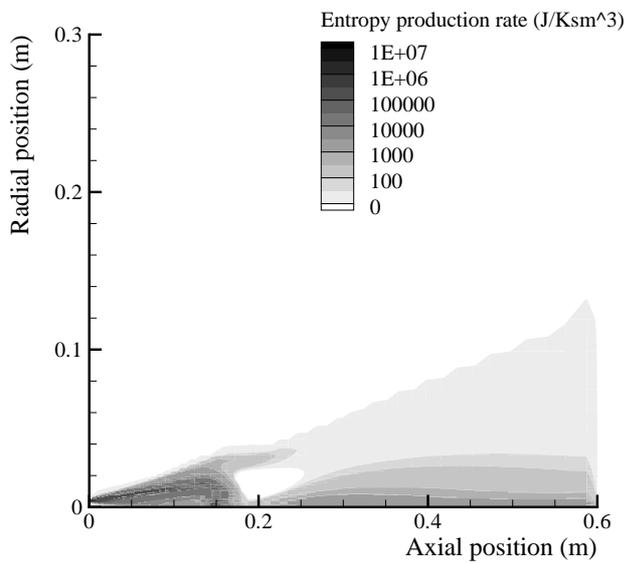


Figure 3: Mean entropy production rate

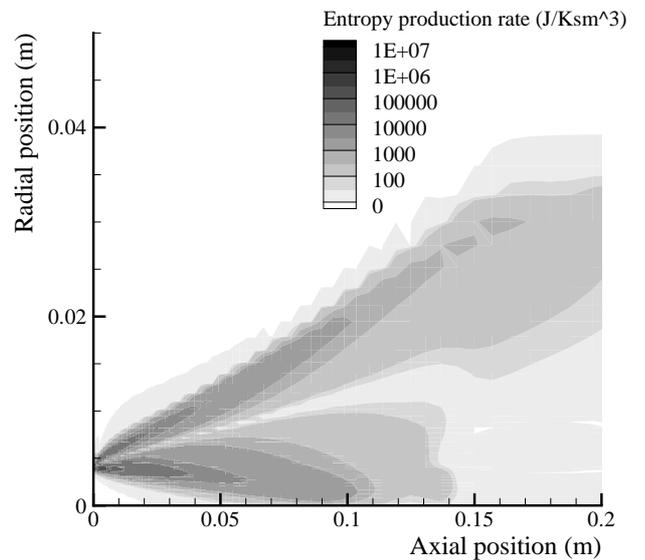


Figure 5: Entropy production due to mean temperature gradients, 2nd term of Eq. (31)

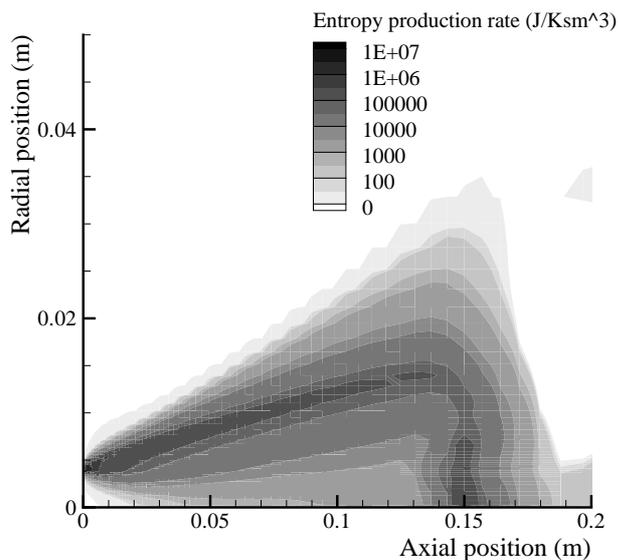


Figure 6: Fine-structure contribution to entropy production model in Eqs. (33)-(35)

RESULTS AND DISCUSSION

The geometry and the simulated mean temperature field of the jet are shown in Fig. 2. This and the species field (not shown) resembled experimental data quite well. The modeled mean entropy production is shown in Figs. 3–4. This is the sum of the contributions from the mean-field, Eq. (31), and from turbulence fine structures, Eqs. (33)-(35). In the former, the heat-flux contribution, that is, the 2nd term of Eq. (31), was by far the largest. This term gave some relatively large local values and is shown in Fig. 5. The major production, however, was found in the fine-structures, shown in Fig. 6. Here, the effects of chemical reactions and pre-reaction mixing are included through the model in Eq. (34). However, the main contributor was the post-reaction mixing term, Eq. (35). This finding corresponds well with the result obtained in [1].

No experimental data are available on entropy production. However, when the volumetric entropy production rate is integrated over the computed domain, it should be comparable to results of an overall entropy balance for the same case. Here, such a balance was evaluated based on the mean values. Then, the sum of entropy inflow to all inflow cells minus the entropy outflow from all outflow cells was 8.62 W/K. The inflow has no concentration fluctuations

and only small temperature fluctuations. In the outlet, these fluctuations will be larger, and hence, the outflow entropy somewhat larger. Thus, the entropy production was somewhat overestimated when using the overall balance based on mean values. Nevertheless, it should be a good indication of the correct result.

The entropy production computed from the model presented above, was 6.14 W/K, or 71 % of that found from the simple balance. The fine-structure model gave 5.88 W/K, of this 2.36 W/K from Eq. (34) and 3.52 W/K from Eq. (35), while the mean-temperature term (Eq. 31) gave 0.25 W/K.

CONCLUDING REMARKS

The Eddy Dissipation Concept (EDC) for turbulent combustion has been extended to include modeling of entropy production. The results obtained are very good when compared with an overall entropy balance of the same case.

REFERENCES

- [1] Dunbar WR, Lior N. (1994) *Combust. Sci. Tech.* 103:41-61, 1994.
- [2] Ertesvåg IS. *Turbulent flow and combustion* (in Norwegian.) Tapir Academic Publisher, Trondheim, Norway, 2000.
- [3] Ertesvåg IS, Magnussen BF. *Comb. Sci. Technol.* 159:213-236, 2000.
- [4] Gran IR, Magnussen BF. *Comb. Sci. Technol.* 119:191-217, 1996.
- [5] Launder BE, Spalding DB, *Comput. Meth. in Appl. Mech. and Eng.* 3:269-289, 1974.
- [6] Magnussen BF, "Modeling of NO_x and soot formation by the Eddy Dissipation Concept," Int. Flame Research Foundation, 1st Topic Oriented Technical Meeting, 17-19 Oct., Amsterdam, Holland, 1989.
- [7] Poinso T, Veynante D. *Theoretical and numerical combustion.* Edwards, Philadelphia PA, 2001.
- [8] Stanciu D, Isvoranu D, Marinescu M, Gogus Y. *Int. J. Appl. Thermodyn.* 4(1):1-18, 2001.
- [9] Teng H, Kinoshita CM, Masutani SM, Zhou J. *ASME J. Energy Resour. Tech.* 120:226-232, 1998.
- [10] Williams F.A. *Combustion theory.* 2nd ed. Benjamin/Cummings Publ. Comp., endthebibliography Menlo Park CA, 1985.