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Analysis of some recently proposed modifications to the Eddy Dissipation Concept (EDC)

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Abstract The widespread use of the Eddy Dissipation Concept (EDC) of Magnussen has led to a number of suggestions to modify the model. These modifications are to a varying extent in agreement with the underlying ideas of EDC. This paper analyzes 20 such attempts. The original formulations of EDC are reviewed and explained. Often, users tend to neglect the expressions for the fraction of reacting fine structures. This part of the model includes some Reynolds number dependency, which is acting where such effects have been requested. The possibly unintended, but widely used, EDC modification in the Ansys Fluent implementation is discussed and analyzed. It is shown that some of the claimed defects of EDC are caused by this implementation. Twelve papers proposing changes of the EDC constants are reviewed and the suggestions analyzed and discussed with respect to the reaction rate, fine-structure model and viscous effects. Models combining Arrhenius and EDC at low turbulence Reynolds numbers and a model based on fractal theory are commented.

Keywords: EDC, turbulent combustion, turbulence-chemistry interaction, model constants, low Reynolds number

1 Introduction

The Eddy Dissipation Concept for turbulent combustion (EDC) by B.F. Magnussen (1981,1989) was initially developed nearly 40 years ago and is widely used in science and engineering. EDC was related to the much simpler Eddy Dissipation Model (EDM) presented by Magnussen and Hjertager (1976), which also can be obtained by simplifying EDC.

The concept appears to be increasingly popular. The main papers (Magnussen, 1989, Gran and Magnussen, 1996, Ertesvåg and Magnussen, 2000) have all got half of their accumulated citations during the last 5-6 years and have been more cited in 2018 than in any previous year (based on scopus.com data as of December 2018). In addition, it seems that several

users cite secondary or tertiary sources for the modeling, either papers by other users or the documentation of a commercial CFD code. Many users just specify "standard EDC" without further information.

During the past decade, quite a few authors have suggested various modifications to EDC. The first one may seem to be Rehm et al. (2009), who proposed to change the constants in the model. Many of these proposals have been made without considering the effects of the modification. In addition, some misunderstandings have been propagated into literature.

The aim of the present paper was to review the proposed modifications and give an analysis of their effects, to explain previous work in a unified way and to examine to which extent the new suggestions agree with the underlying ideas of EDC. My background is as a student (1980s), co-worker (1990s, early 2000s) and successor of professor Magnussen at NTNU. EDC and its formulations have been presented previously. Some elements relevant for the discussions are repeated below. The most comprehensive presentation is found in the textbook (Ertesvåg, 2000/2008), while the main papers are listed and partly available at the web site `folk.ntnu.no/ivarse/edc`.

The main idea of EDC is that chemical reactions in turbulent flows occur in intermittent fine structures or small eddies. The species gradients and molecular mixing coexist with the velocity gradients, that is, viscous dissipation. Briefly described, the Eddy Dissipation Concept consists of a cascade model and a reactor model. The cascade model links the fine structures, where reactions are assumed to occur, to the mean turbulence field, resolved by RANS, and was initially outlined in private notes of Magnussen in 1975. The resulting expressions were used in EDC by Magnussen (1981), while discussed and reformulated in the doctoral thesis (Ertesvåg, 1991) and further discussed by Ertesvåg and Magnussen (2000). These smaller eddies are regarded as a reactor, and the reaction rate is formulated from the species mass balance for this reactor (Magnussen, 1981, 1989, Gran and Magnussen, 1996).

The outline of the paper is as follows: In the next sections, an overview of EDC will be given, and expressions for the fine-structure and reacting mass fractions will be reviewed and analyzed for use in the following sections. In Sect. 4 the discussion of the 2nd EDC constant will

be revisited and updated, due to queries in literature. Section 5 will describe and analyze the anonymous modification of EDC in the Ansys Fluent implementation. Furthermore, deductions on EDC in literature based on this modification will be discussed. The simple way to modify a model is to change constants. Twelve papers proposing such changes will be reviewed in Sect. 6, and effects and consequences analyzed. In Sect. 7 some other modifications will be discussed, including one based on fractal theory. Specific discussions will be given in each section, before an overall discussion and eventually, some concluding remarks.

2 Overview of EDC

2.1 Reaction rates

The approach of EDC is to solve partial differential or "transport" equations for the mean mass of individual species. Hence, the mean reaction rates have to be expressed.

The reaction rate of EDC results from a mass balance for the fine-structure reactor, as described by Magnussen (1981, 1989). The inflow has the properties of the "surroundings" (denoted by ^{o}) of the fine-structure reactor, while the interior and the outflow have the fine-structure properties (denoted by *), Fig. 1. Fig. 1

The mass inflow rate divided by the mass of the fine structures is denoted by $\dot{m}^*$. This can also be regarded as a time scale, $\tau^* = (\dot{m}^*)^{-1}$. The mass balance of the reactor gives a reaction rate for the reactor,

$$R_k^* = \rho^* \dot{m}^* (Y_k^* - Y_k^o). \tag{1}$$

The ratio of mass in fine structures to the total mass is represented by γ^*. The intermittent fine structures are assumed to be gathered in certain regions of the total flow, in particular in the interface between the bigger eddies. The ratio of mass in these fine-structure containing regions to the total mass is denoted by γ_λ. Furthermore, it is assumed that not all the small eddies have conditions that favor reactions to proceed. Therefore, the quantity χ denotes the fraction of the fine structures that reacts. Accordingly, $\gamma^*\chi$ is the reactor mass as a fraction

of the total mass. The relations between χ, γ_λ and γ^* will be discussed below. However, the recommended relation among the latter two is $\gamma^* = \gamma_\lambda^2$ (Magnussen, 2005).

The reactions are assumed to occur in the fine structures, and the mean reaction rate is expressed as

$$\overline{R}_k = \frac{\bar{\rho}}{\rho^*}\gamma^*\chi R_k^*, \tag{2}$$

which leads to

$$\overline{R}_k = \frac{\bar{\rho}\gamma^*\chi}{\tau^*}(Y_k^* - Y_k^o). \tag{3}$$

A mean mass fraction is a mass-weighted average of the fine-structure reactor and its surroundings,

$$\widetilde{Y}_k = \gamma^*\chi Y_k^* + (1 - \gamma^*\chi)Y_k^o. \tag{4}$$

Accordingly,

$$(Y_k^* - Y_k^o) = \frac{Y_k^* - \widetilde{Y}_k}{(1 - \gamma^*\chi)} \tag{5}$$

can be introduced in Eq. 3.

2.2 Fine structures model

The fine-structure length and velocity scales were developed from the cascade model (Magnussen, 1981, Ertesvåg and Magnussen, 2000) and expressed as

$$L^* = \frac{2}{3}\left(\frac{3C_{\mathrm{D2}}^3}{C_{\mathrm{D1}}^2}\right)^{1/4}\left(\frac{\nu^3}{\varepsilon}\right)^{1/4} \tag{6}$$

and

$$u^* = \left(\frac{C_{\mathrm{D2}}}{3C_{\mathrm{D1}}^2}\right)^{1/4}(\nu\varepsilon)^{1/4}. \tag{7}$$

These scales are of the same order of magnitude as the Kolmogorov scales, η and v, which are recognized in the non-constant parts of the expressions. The corresponding Reynolds number

becomes

$$Re^* = \frac{u^* L^*}{\nu} = \frac{2C_{\mathrm{D2}}}{3C_{\mathrm{D1}}}. \tag{8}$$

Furthermore, the length and velocity scales were used (Magnussen, 1981) to formulate the expressions

$$\gamma_\lambda = \left(\frac{3C_{\mathrm{D2}}}{4C_{\mathrm{D1}}^2}\right)^{1/4} \left(\frac{\nu\varepsilon}{k^2}\right)^{1/4} = C_\gamma \, Re_{\mathrm{T}}^{-1/4} \tag{9}$$

and

$$\tau^* = (\dot{m}^*)^{-1} = \left(\frac{C_{\mathrm{D2}}}{3}\right)^{1/2} \left(\frac{\nu}{\varepsilon}\right)^{1/2} = C_\tau \left(\frac{\nu}{\varepsilon}\right)^{1/2}, \tag{10}$$

where the single-symbol constants C_γ and C_τ have been introduced for convenience and discussion. The mean reaction rate contains the product γ_λ^2/τ^*, which can be expressed as

$$\frac{\gamma_\lambda^2}{\tau^*} = \frac{3}{2C_{\mathrm{D1}}} \frac{\varepsilon}{k} = C_R \frac{\varepsilon}{k} = \frac{C_\gamma^2}{C_\tau} \frac{\varepsilon}{k}. \tag{11}$$

Here, the symbol C_R was introduced for $(3/(2C_{\mathrm{D1}}))$, and in the third equality, the constants C_γ and C_τ from Eqs. 9 and 10 were used. With the original values of the primary constants $C_{\mathrm{D1}} = 0.135$ and $C_{\mathrm{D2}} = 0.50$, the secondary constants take the values $C_\gamma = 2.1377$, $C_\tau = 0.4082$ and $C_R = 11.1$.

3 The fine-structure and reacting mass fractions

3.1 Development over time

The first appearance of χ and γ^* seems to have been at the 1978 Combustion Symposium (Magnussen et al., 1978), where the quantities were introduced in the Eddy Dissipation Model of Magnussen and Hjertager (1976). Next, the distinction and weighting between "surroundings" and "reactor" values appeared in Magnussen (1980). The papers mentioned in the following are accessible to a varying degree, from journal articles to relatively obscure scientific meeting papers. The latter are mentioned when they are the first occurrence of an element of the model.

In the widely known version of Magnussen (1981), $\gamma_\lambda = (\gamma^*)^{1/3}$ was introduced. The reacting fraction χ was expressed as

$$\chi = \frac{\widetilde{Y}_{\rm pr}/(1+r)}{\gamma_\lambda(\widetilde{Y}_{\rm pr}/(1+r) + \widetilde{Y}_{\rm fu})} = \frac{1}{\gamma_\lambda}\chi' \tag{12}$$

and the mean reaction rate as

$$\overline{R}_k = -\frac{\bar{\rho}\dot{m}^*\gamma^*\chi}{1-\gamma^*\chi}(\widetilde{Y}_k - Y_k^*) = -\frac{\bar{\rho}\dot{m}^*\gamma_\lambda^2\chi'}{1-\gamma_\lambda^2\chi'}(\widetilde{Y}_k - Y_k^*). \tag{13}$$

Here, and in the following, the symbol χ' has been introduced to separate γ_λ from the mass-fraction containing part of χ, cf. Eq. 12. For infinitely fast reactions, the fuel reaction rate, $\overline{R}_{\rm fu}$, is expressed by replacing $(\widetilde{Y}_k - Y_k^*)$ in Eq. 13 by $\widetilde{Y}_{\rm min} = \min(\widetilde{Y}_{\rm fu}, \widetilde{Y}_{\rm ox}/r)$.

During the 1980s, various formulations of χ were tried, Magnussen (1985), Brostrøm (1987) (doctoral student of Magnussen), before it was more or less settled by Magnussen (1989). This version was used by Gran (1994) to implement detailed chemical mechanisms. Following Gran (1994), Gran and Magnussen (1996), the 1989 version can be formulated as

$$\chi = \chi_1 \cdot \chi_2 \cdot \chi_3, \tag{14}$$

$$\chi_1 = \frac{\left(\widetilde{Y}_{\rm min} + \widetilde{Y}_{\rm pr}/(1+r)\right)^2}{\left(\widetilde{Y}_{\rm fu} + \widetilde{Y}_{\rm pr}/(1+r)\right)\left(\widetilde{Y}_{\rm ox}/r + \widetilde{Y}_{\rm pr}/(1+r)\right)}, \tag{15}$$

$$\chi_2 = \min\left\{\frac{1}{\gamma_\lambda}\cdot\frac{\widetilde{Y}_{\rm pr}/(1+r)}{\widetilde{Y}_{\rm pr}/(1+r) + \widetilde{Y}_{\rm min}}, 1\right\} = \min\left\{\frac{1}{\gamma_\lambda}\cdot\chi_2', 1\right\}, \tag{16}$$

$$\chi_3 = \min\left\{\frac{\gamma_\lambda\left(\widetilde{Y}_{\rm pr}/(1+r) + \widetilde{Y}_{\rm min}\right)}{\widetilde{Y}_{\rm min}}, 1\right\} = \min\left\{\gamma_\lambda\cdot\chi_3', 1\right\}. \tag{17}$$

In this version, the relation $\gamma^* = \gamma_\lambda^3$ was maintained, while a factor γ_λ^{-1} was introduced. The reaction rate now was expressed as

$$\overline{R}_k = -\frac{\bar{\rho}\dot{m}^*\gamma^*(\chi/\gamma_\lambda)}{1-\gamma^*\chi}(\widetilde{Y}_k - Y_k^*) = -\frac{\bar{\rho}\dot{m}^*\gamma_\lambda^2\chi}{1-\gamma_\lambda^3\chi}(\widetilde{Y}_k - Y_k^*). \tag{18}$$

The expressions of Eqs. 14-17 can, in principle, be formulated for each reaction of a multi-step mechanism. However, Gran and Magnussen (1996) used the single-step global reaction of fuel and oxygen to final product to formulate a single χ used in Eq. 18 for all species of a multi-step chemical mechanism. This seems to be the practice of other users as well.

The most recent formulation was presented by Magnussen (2002b,2005), with the χ formulated as

$$\chi = \frac{\widetilde{Y}_{\rm pr}/(1+r)}{(\widetilde{Y}_{\rm pr}/(1+r) + \widetilde{Y}_{\rm min})}. \tag{19}$$

A notable feature was a reformulation of γ^* into $\gamma^* = \gamma_\lambda^2$, i.e. square rather than cube. The reaction rate now became

$$\overline{R}_k = -\frac{\overline{\rho}\dot{m}^*\gamma^*\chi}{1-\gamma^*\chi}(\widetilde{Y}_k - Y_k^*) = -\frac{\overline{\rho}\dot{m}^*\gamma_\lambda^2\chi}{1-\gamma_\lambda^2\chi}(\widetilde{Y}_k - Y_k^*) \tag{20}$$

The resemblance between the last term of Eq. 20 and the last term of Eq. 13 should be noted. Formally, except for the χ, the only change from the 1989 version was in the denominator, where the square of γ_λ replaces the cube of it. In most cases this even seems to have little or modest influence on the results.

The overall expressions of Eqs. 19-20 were formally identical to those of Magnussen (1985, 2002a). However, the interpretations were different, as γ^* still was γ_λ^3, while χ included the reciprocal of γ_λ. Accordingly, the product $\gamma^*\chi$ was the same in 1985, 2002 and 2005.

The conceptual modification was, however, more notable. From 1978, the fine-structure mass fraction had been modeled as $\gamma^* = (u^*/u')^3$, where u' and u^* are the velocity scales of turbulence and the fine structures, respectively. This corresponds to a sheet-like structure of the small scales (known as Corrsin's model). The introduction of the factor γ_λ^{-1} at different places and different points of the history, was explained by other considerations. Now, with the model $\gamma^* = (u^*/u')^2$ for the fine-structure mass fraction, the interpretation changed to a tube-like structure (Tennekes' model).

When using a detailed mechanism, Gran (1994), Gran and Magnussen (1996) compared χ of

Eqs. 14-17 to the simple form $\chi = 1$. The differences in the tested cases were modest and, due to its simplicity, $\chi = 1$ was chosen. The argument was that the solution of the chemical reactor with detailed chemistry would determine whether and to what extent the reaction occurred. An alternative interpretation of this could be that the quantity $\chi(Y_k^o - Y_k^*)$ was solved from the reactor, rather than $(Y_k^o - Y_k^*)$. That is, χ was not unity but became a part of the solution.

3.2 Analysis of the χ expressions

A comparison of the different formulations of χ can be made easier by expressing the three mass fractions $\widetilde{Y}_{\rm fu}$, $\widetilde{Y}_{\rm ox}$ and $\widetilde{Y}_{\rm pr}$ from two parameters: The mixture fraction and the extent of reaction, here denoted f and c, which both take values in the range (0,1).

The mixture fraction f can be understood as the fraction of the local mass that originates from the fuel inlet. For a perfectly premixed flow, this is a constant value. For a stoichiometric mixture, $f = f_{\rm st} = 1/(1 + r)$.

The extent of reaction, c, can take any value from 0, for no reaction, to 1 for maximum fuel reaction. In lean flames, all the fuel has reacted in a complete reaction. In rich flames, lack of oxygen limits reaction, and the maximum fraction of reacted fuel is $(1-f)/(rf)$, which equals the ratio of the actual to the stoichiometric amount of oxidizer for the fuel. This quantity is known as the excess-air ratio, λ, or the reciprocal of the equivalence ratio.

In this context, the f and c are just parameters describing the local mixture. No assumptions are made regarding their role as characteristic variables in the model (cf. "presumed pdf" or "flamelet" models).

From a given set of (f,c), the composition can be determined as

$$\widetilde{Y}_{\rm pr} = c \cdot \min(1, (1 - f)/(rf)) \cdot (1 + r)f, \tag{21}$$

$$\widetilde{Y}_{\rm fu} = f - \widetilde{Y}_{\rm pr}/(1 + r), \tag{22}$$

$$\widetilde{Y}_{\rm ox} = (1-f) - r\widetilde{Y}_{\rm pr}/(1+r). \tag{23}$$

Furthermore,

$$\widetilde{Y}_{\rm min} = \begin{cases} \widetilde{Y}_{\rm fu} = (1-c)f & \text{for } f \le f_{\rm st} \\ \frac{1}{r}\widetilde{Y}_{\rm ox} = \frac{1}{r}(1-c)(1-f) & \text{for } f \ge f_{\rm st}. \end{cases} \tag{24}$$

From the expressions above, any of the χ (or χ') expressions can be found as a function of (f,c). It can be shown that the 2005 version, Eq. 19, gives $\chi = c$, independent of f. For lean flames, $f \le f_{\rm st}$, this is also the result for the χ' from 1981, Eq. 12, while for rich flames, $\chi' = (1-f)/(rf) = \lambda$.

In the 1989/94 version (see Eqs. 14-17),

$$\chi_1 = \left\{ \begin{array}{ll} rf/(1-f) = \lambda^{-1} & \text{for } f < f_{\rm st} \quad (\lambda > 1) \\ 1 & \text{for } f = f_{\rm st} \quad (\lambda = 1) \\ (1-f)/(rf) = \lambda & \text{for } f > f_{\rm st} \quad (\lambda < 1), \end{array} \right\} = \min\{\lambda^{-1}, \lambda\}, \tag{25}$$

$$\chi_2 = \min\left\{(c/\gamma_\lambda), 1\right\}, \tag{26}$$

$$\chi_3 = \min\left\{\gamma_\lambda/(1-c), 1\right\}. \tag{27}$$

It is seen that χ_1 (Eq. 25) is independent of the reaction progress and dependent only on the mixture, while the two other factors depend on the extent of reaction alone, and are independent of the local stoichiometry. For rich flames ($f > f_{\rm st}$), χ_1 equals the χ' from 1981.

The quantity χ_2 takes non-unity values only at small values of the extent of reaction c, i.e. at $c < \gamma_\lambda$. For values of c where both $c > \gamma_\lambda$ and $c > (1-\gamma_\lambda)$, the product $\chi_2 \cdot \chi_3$ approaches unity. At $c = 1$ for any f, the product $\chi_2 \cdot \chi_3 = 1$. On the other hand, at small values of c, where both $c < \gamma_\lambda$ and $c < (1-\gamma_\lambda)$, the product $\chi_2 \cdot \chi_3$ approaches c.

Fig. 2

In Fig. 2, χ' ($= \gamma_\lambda \chi$) of the 1981 version, Eq. 12, and χ of the 1989 version, Eqs. 14-17, are compared for two values of c and (for 1989) two values of $Re_{\rm T}$. The values 800 and 70 correspond to γ_λ values of, respectively, 0.40 and 0.74. Fuel and oxidizer were methane and air, hence $r = 17.16$ and $f_{\rm st} = 0.0551$. The graph is shown for f from 0 to 0.2. For larger

values, all curves continued smoothly to $\chi = 0$ at $f = 1$. As mentioned above, the 2005 version gave $\chi = c$, independent of f, and equaled the χ' of 1981 for $f < f_{\rm st}$.

Effects of turbulence Reynolds number

Since χ_2 and χ_3 are functions of γ_λ, Eqs. 16-17 or Eqs. 26-27, they are also functions of the turbulence Reynolds number. χ_2 has below-unity values at low Reynolds numbers, and the lower $Re_{\rm T}$ limit for a unity χ_2 value decreases with increasing c. χ_3 is unity at low values of $Re_{\rm T}$, and the $Re_{\rm T}$ limit for a non-unity value increases with the extent of reaction c. For a given value of c, the value of χ_3 is reduced with increasing $Re_{\rm T}$. Fig. 3

Figure 3 shows the product $\chi_2\chi_3$ as a function of turbulence Reynolds number $Re_{\rm T}$ for values of c ranging from 0.4 to 0.8. This graph demonstrates that the χ expression of 1989 includes a low-Reynolds-number modification of the reaction rate for finite-rate reactions. Also at high Reynolds numbers, the reaction rate is reduced. For moderate $Re_{\rm T}$ and a high extent of reaction, the product is $\chi_2\chi_3 = 1$.

Fast chemistry approximations

When using the fast chemistry assumption ("mixed is burnt"), all reactants that can react, are assumed to have reacted. The effects on the various χ and reaction rate expressions can be investigated from the expressions above, with $c = 1$.

The 2005 version, Eq. 19, simplifies to $\chi = 1$.

The 1981 version, Eq. 12, gives

$$\chi' = \begin{cases} 1 & \text{for } f \le f_{\rm st} \quad (\lambda \ge 1) \\ (1-f)/(rf) = \lambda & \text{for } f > f_{\rm st} \quad (\lambda < 1), \end{cases} \tag{28}$$

In the 1989/1994 version, both $\chi_2 = 1$ and $\chi_3 = 1$. Hence, χ from Eqs. 14-17 becomes equal to χ_1 of Eq. 25. That is, $\chi = \min\{\lambda^{-1}, \lambda\}$.

3.3 Use of χ and γ_λ in the reaction rate

For the discussion, it can be convenient to define an "EDC factor" g_{EDC} such that

$$\overline{R}_k = g_{\mathrm{EDC}} \frac{\bar{\rho}}{\tau^*}(Y_k^* - \widetilde{Y}_k). \tag{29}$$

Since the 1981 formulation of χ included γ_λ as a divisor, it can be written as $\chi = \chi'/\gamma_\lambda$ as shown in Eq. 12. The EDC factor of Eq. 13 then turns out as

$$g_{\mathrm{EDC81}} = \frac{\gamma_\lambda^2 \chi'}{1 - \gamma_\lambda^2 \chi'}. \tag{30}$$

In the 1989/1994 version, the reciprocal of γ_λ appeared as a factor in the reaction rate expression, separated from χ. Hence, with Eq. 18 the EDC factor became

$$g_{\mathrm{EDC89}} = \frac{\gamma_\lambda^2 \chi}{1 - \gamma_\lambda^3 \chi}. \tag{31}$$

Here, Gran (1994) suggested $\chi = 1$ as an alternative to simplify the calculations:

$$g_{\mathrm{EDC94}} = \frac{\gamma_\lambda^2}{1 - \gamma_\lambda^3}. \tag{32}$$

In the 2005 version (Magnussen, 2005), the fine-structure mass fraction was re-interpreted as $\gamma^* = \gamma_\lambda^2$, and the reciprocal of γ_λ was removed from the reaction rate expression, Eq. 20. Hence

$$g_{\mathrm{EDC05}} = \frac{\gamma_\lambda^2 \chi}{1 - \gamma_\lambda^2 \chi}. \tag{33}$$

That is, similar to Eq. 30 although with different χ formulations. Furthermore, as mentioned above, versions presented by Magnussen (1985,2002a) were formally identical to 2005, albeit without the re-interpretation of γ^*.

The different formulations of the EDC factor, with and without unity χ, can be compared with the re-expressions of χ in terms of the local excess air ratio (λ) and extent of reaction

(c) shown above. Fig. 4

Figure 4 shows three versions of the factor with unity χ. It should be noted that the third of these, $\gamma_\lambda^3/(1-\gamma_\lambda^3)$, has not been suggested or used by Magnussen or his co-workers. It is however, tried by others (Li et al., 2017, Bösenhofer et al., 2018) with the label "EDC1981". Furthermore, the factor of Eqs. 30 and 33 with (non-unity) χ from 1994 is shown together with Eq. 31 with the same χ. Here, the local composition was set by $\lambda = 0.9$ and $c = 0.6$. Figure 5 shows the same factor for some values of c. It is seen that for uncompleted reactions (finite rate reactions), the inclusion of χ reduces the reaction rate, in particular at low Re_T. More deviation from stoichiometry will reduce χ_1 as shown above, Eq. 25. Fig. 5

The graphs demonstrates that the EDC factor can exceed unity at low Reynolds numbers. Practically, this can be handled by setting an upper limit either to the EDC factor or to γ_λ.

3.4 Intermediate discussion

The history of EDC indicates that there were some struggles with the interpretations and formulations of the fine-structure and reacting mass fractions, γ^* and χ. The cube formulation corresponds to a sheet-like structure of the fine structures (Corrsin's model), while the square formulation corresponds to a tube-like structure (Tennekes' model). The latter was depicted as an illustration by Magnussen (1985, 1989), although the former was formulated. Moreover, the feature that a χ including the reciprocal of γ_λ readily exceeds unity, was disturbing since this should be a fraction of something. In spite of this, the reciprocal of γ_λ appeared in all versions before 1987 (Magnussen et al., 1978, Magnussen, 1980, 1981, 1985), when Brostrøm (1987) - doctoral student of Magnussen - tried to limit it to unity, leading to the 1989 formulation. The 2005 version settled both the problem of the fine structure interpretation and of the not-above unity χ. Evaluated in aftermath, a reasonable interpretation seems to be that Eq. 33 is the formulation that should have been there all the time.

If a recommendation should be given, this can be that Eq. 20 with χ from Eqs. 14-17 can be applied. These satisfy the conceptual requirements, they are tested in literature (e.g.

Gran and Magnussen, 1996, Lilleberg et al., 2013) more than the other formulations (but $\chi = 1$), and they seem to provide some of the requested effects for low Re_{T} and diluted flames (Lewandowski and Ertesvåg, 2018). However, there might be a potential in improving the expression for χ. On the other hand, Magnussen has advocated the simplicity of formulations, thus suggesting Eq. 19.

4 Decaying turbulence and the 2nd EDC constant

It has been indicated (e.g. Aminian et al., 2012) that the discussion of the 2nd EDC constant C_{D2} was insufficient. This section can be viewed as a comment to this, based on newer literature.

The constants of the cascade model originated from 1975 (private notes of B.F. Magnussen) and were used in the first version of EDC (Magnussen, 1981). The development was discussed by Ertesvåg (1991). There, a revised formulation and development was presented, while the numerical values were kept. Further discussion was given by Ertesvåg and Magnussen (2000).

The cascade can be viewed as a dissipation model,

$$-\frac{dk}{dt} = \varepsilon = C_{\mathrm{D1}}\omega k + C_{\mathrm{D2}}\nu\omega^2. \tag{34}$$

The quantity ω is a strain rate or frequency. A 2nd equation can be formulated for this quantity, with inertial and viscous destruction terms similar to those of Eq. 34. The two equations will describe decaying isotropic turbulence at the level of Reynolds Averaged Navier Stokes, RANS. This case has been used to determine the constant(s) of the decay terms of most or all RANS turbulence models.

In this flow case, experimental and theoretical results show that the turbulence energy will decay as $k \sim t^{-n}$. The two constants of the 2nd equation can be settled by the decay exponent n at, respectively, very high and very low turbulence Reynolds numbers.

Perot and de Bruyn Kops (2006) have contributed to the topic by formulating a k-λ model,

where the 2nd quantity λ was the reciprocal of a length scale. The dissipation was expressed as

$$\varepsilon = \alpha_H \lambda k^{3/2} + \alpha_L \nu \lambda^2 k. \tag{35}$$

For both models, the constant of the inertial term, $C_{\mathrm{D1}} = 0.135$ or $\alpha_H = 1$, was determined from other considerations. The remaining constant, C_{D2} or α_L, can be related to the transition from the high Re_{T} limit to the low Re_{T} limit. This transition depends on the ratio $C_{\mathrm{D2}}/C_{\mathrm{D1}}^2$ or α_L/α_H^2.

Since 1991/2000, more data have become available, in particular from DNS. These were utilized in the discussion of Perot and de Bruyn Kops (2006). They noted that the transition was "not highly sensitive" to the ratio of the constants, and recommend the value $\alpha_L = 15$ (with $\alpha_H = 1$), which corresponds to a value of $C_{\mathrm{D2}} = 0.27$ (with $C_{\mathrm{D1}} = 0.135$). Apparently, the moderate sensitivity had limits. It seemed that variation outside their range of trial values, α_L from 6 to 50, would clearly be outside the domain of available data. This corresponded to limits of C_{D2} at 0.11 and 0.91. The original value of $C_{\mathrm{D2}} = 0.50$ corresponded to $\alpha_L = 27.4$, which was well inside the variation.

The power-law exponent n can be found from the two model equations. The constants appearing in the 2nd (ω or λ) equation were determined by the limiting decay exponent n at, respectively, very high and very low turbulence Reynolds numbers. These exponents were tabulated by Perot and de Bruyn Kops (2006). Fig. 6

Figure 6 shows the power law exponent from the two models with a selection of α_L or C_{D2} values. The high and low Re_{T} limits corresponded to data for a κ^2 low wavenumber spectrum. This graph was made to be directly comparable to Fig. 2 of Perot and de Bruyn Kops (2006).

For the discussion below (Sect. 6), it was noted that $C_{\mathrm{D2}}/C_{\mathrm{D1}}^2 = 4C_\gamma^4/3$ and that the C_{D2} range of 0.11 to 0.91 (α_L from 6 to 50) corresponded to a range of C_γ from 1.46 to 2.47.

Another visualization of the transition from the inertial to the viscous dissipation term can be to compare the viscous term to the total dissipation. For the discussion, with the expressions above, the turbulence Reynolds number at a certain ratio of the viscous term ($\varepsilon_2 = C_{\mathrm{D2}} \nu \omega^2$)

to the total dissipation, was expressed as

$$Re_{\mathrm{T}} = \frac{(1-\varepsilon_2/\varepsilon)^2}{\varepsilon_2/\varepsilon}\frac{C_{D2}}{C_{D1}^2}. \tag{36}$$

Resolved, this expression gives one positive root for the ratio $\varepsilon_2/\varepsilon$. The relation can also be found from the model of Eq. 35, with constants α_L/α_H^2 replacing $C_{\mathrm{D2}}/C_{\mathrm{D1}}^2$. Fig. 7

The ratio of the viscous term to the total dissipation is shown in Fig. 7 for the same constants as in Fig. 6. The corresponding values of C_γ are also included.

Decaying turbulence is relevant for combustion because it is a case where viscous forces are important and which can be modeled. It can be seen together with models and data for the viscous part of the spectrum, as discussed by Ertesvåg and Magnussen (2000). Decaying turbulence is also used for determination of constants or functions of turbulence models. Some flexibility has been practiced, however, in settling the model constants and functions, to compensate for imperfectness of the models. For instance, the high Reynolds number decay indicated an exponent of 1.2-1.3, which corresponded to $C_{\varepsilon 2}$ of about 1.80, while the "standard" value adopted for the k-ε model was 1.92 (Launder and Spalding, 1974).

5 Fine-structure reactors: The Ansys Fluent modification

5.1 The EDC fine-structure reactor and species reaction rate

Gran (1994), Gran and Magnussen (1996) implemented multi-step finite-rate chemistry with EDC by treating the fine structure as a homogeneous reactor, also called a (transient) perfectly stirred reactor (PSR). This is a transient reactor with inflow and outflow, where the outflow properties are equal to those inside the reactor. The reactor species mass balance can be written as

$$\frac{dY_k^*}{dt} = \frac{1}{\rho^*}R_k(T^*, Y_j^*) + \frac{1}{\tau^*}(Y_k^o - Y_k^*). \tag{37}$$

Here, the reaction rate R_k is expressed from the reactor temperature and composition. In

case of steady state, solution of the equation leads to Eq. 1 with $R_k^* = R_k(T^*, Y_j^*)$,

$$(Y_k^* - Y_k^o) = \frac{R_k^*}{\rho^*}\tau^* \tag{38}$$

and, subsequently, to the mean reaction rate

$$\overline{R}_k = \frac{\bar{\rho}\gamma_\lambda^2\chi}{\tau^*}(Y_k^* - Y_k^o). \tag{39}$$

5.2 The Ansys Fluent implementation of the reactor of EDC

A popular commercial CFD code, in which EDC is implemented, is Ansys Fluent. Their implementation was slightly different from that described above, as an isobaric batch reactor (BaR) was used to represent the fine structures (Ansys, 2016a,b). This is sometimes (e.g. De et al., 2011, Li et al., 2017) presented as a plug flow reactor (PFR), which with constant flow velocity and cross-sectional area can be transformed to a time-dependent batch reactor. The initial and final properties of the batch reactor then correspond to the inlet and outlet of the PFR. In the transient form, the species mass balance can be expressed as

$$\frac{dY_k}{dt} = \left(\frac{R_k}{\rho}\right)_{\text{BaR}}. \tag{40}$$

In the Fluent implementation, Eq. 40 was integrated from $Y_k(t=0) = \widetilde{Y}_k$, "the current species and temperature of the cell" (Ansys, 2016a, Sect. 7.1.2.5), to $Y_k(t=\tau^*) = Y_k^*$, giving

$$(Y_k^* - \widetilde{Y}_k) = \int_0^{\tau^*} \left(\frac{R_k}{\rho}\right)_{\text{BaR}} dt = \frac{R_k^*}{\rho^*}\tau^*. \tag{41}$$

This implies that the mean values were taken as initial/inlet values. Introducing this reactor reaction rate R_k^* into Eq. 2 gives an expression of the mean reaction rate.

The two approaches leading to Eqs. 38 and 41 have similarities, but also differences. The ratio of the resulting mean reaction rates can be expressed as

$$F = \frac{\overline{R}_{k,\text{meaninlet}}}{\overline{R}_{k,\text{surr.inlet}}} = \frac{(Y_k^* - \widetilde{Y}_k)}{(Y_k^* - Y_k^o)} = 1 - \gamma^* \chi, \tag{42}$$

where Eq. 5 was used in the last equality.

Here, it is noted that in the Fluent implementation, χ is always set to unity. Including this aspect in the discussion, the ratio becomes

$$F = \frac{\overline{R}_{k,\text{meaninlet}}(\chi = 1)}{\overline{R}_{k,\text{surr.inlet}}} = \frac{1}{\chi}(1 - \gamma^* \chi) \tag{43}$$

For the discussion, four different versions can be considered: First, in the version implemented into Fluent, $\gamma^* = \gamma_\lambda^3$ and $\chi = 1$. This is a version used outside Fluent, as well. Then,

$$F = F_1 = 1 - \gamma_\lambda^3. \tag{44}$$

Second, the expression could be $\gamma^* = \gamma_\lambda^2$ (with $\chi = 1$), hence

$$F = F_2 = 1 - \gamma_\lambda^2. \tag{45}$$

Third, a non-unity χ from Eqs. 14–17 or Eqs. 25–27 can be included. The ratio, Eq. 43, with $\gamma^* = \gamma_\lambda^3$ and $\gamma^* = \gamma_\lambda^2$, respectively, becomes

$$F = F_3 = \frac{1}{\chi}(1 - \gamma_\lambda^3 \chi) \tag{46}$$

and

$$F = F_4 = \frac{1}{\chi}(1 - \gamma_\lambda^2 \chi). \tag{47}$$

Fig. 8

The four ratios are shown in Fig. 8 together with χ (for $\lambda = 0.9$, $c = 0.50$ in Eqs. 25–27). When F is above unity, the mean-inlet implementation overpredicts the mean reaction rate compared to the conventional implementation with the surroundings inlet.

For moderately high Reynolds numbers, the ratio is close to unity. That is, if χ is set to unity.

At low Reynolds numbers, the Fluent implementation reduces the reaction rate. However, compared to a version with a non-unity χ, the reduction is less. For cases with a reaction deviating from stoichiometry, the effect can be an increased reaction rate in Fluent.

A recent study by Lewandowski and Ertesvåg (2018) showed that the differences were notable in temperature of the reacting zone of the Delft jet-in-hot-coflow flame.

It should be noted that the present comparison concerned the differences caused by use of the mean value as inflow rather than the surroundings value. The BaR/PFR vs. PSR differences, which also exist, have to be visualized with other assumptions.

A question that remains, due to missing documentation, is how the Fluent modification was motivated and whether it was intended at all. It can be traced back to a conference paper by Jessee et al. (1993), who did a similar implementation, however, without explanation or comparison.

5.3 Low-Reynolds number limit of validity

De et al. (2011) claimed to demonstrate that the validity of EDC is limited to $Re_{\mathrm{T}} > 65$. The arguments were as follows:

The mean reaction rate was expressed following Gran and Magnussen (1996), Eq. 18 with $\chi = 1$, as

$$\overline{R}_k = \frac{\overline{\rho}\gamma_\lambda^2}{\tau^*(1-\gamma_\lambda^3)}(Y_k^* - \widetilde{Y}_k). \tag{48}$$

Here, De et al. (2011) introduced the time scale τ_{mix} for discussion purposes,

$$\frac{1}{\tau_{\mathrm{mix}}} = \frac{\gamma_\lambda^2}{(1-\gamma_\lambda^3)}\frac{1}{\tau^*} = \frac{1}{(1-\gamma_\lambda^3)}\frac{C_\gamma^2}{C_\tau}\frac{1}{\theta}, \tag{49}$$

where $\theta = k/\varepsilon$ is the large-scale mixing or energy-turnover timescale. This corresponds to Eq. 10 of De et al. (2011). With a ratio of the two time scales introduced as (their Eq. 12),

$$R = \frac{\tau^*}{\tau_{\mathrm{mix}}} = \frac{\gamma_\lambda^2}{(1-\gamma_\lambda^3)}, \tag{50}$$

Eq. 48 now can be expressed as

$$\frac{\overline{R}_k}{\overline{\rho}} = \frac{R}{\tau^*}(Y_k^* - \widetilde{Y}_k). \tag{51}$$

Next, from the Fluent implementation with Eq. 41,

$$\frac{R_k^*}{\rho^*} = \frac{1}{\tau^*}(Y_k^* - \widetilde{Y}_k). \tag{52}$$

The species difference $(Y_k^* - \widetilde{Y}_k)$ is the same in Eqs. 51 and 52. Based on these relations it was argued that the time scale for small-scale (fine-structure) exchange, τ^*, should be less than the time scale of the large-scale exchange, $\tau_{\rm mix} = \tau^*/R$. Hence, $R < 1$ or $\gamma_\lambda^2 < (1-\gamma_\lambda^3)$, which gave the limits $\gamma_\lambda < 0.75$ and $Re_{\rm T} > 65$.

The development above is plausible, however, with an important reservation: The Fluent use of batch/plug-flow reactor with average conditions as initial/inlet values is a deviation from the conventional EDC. Equation 41 cannot be introduced into Eq. 2 to obtain the mean reaction rate, Eq. 48.

In EDC, the inflow to the reactor has the conditions of the surroundings (Y_k^o). Therefore, the fine-structure reaction rate should, instead of Eq. 41, be Eq. 38, which also can be regarded as Eq. 40 integrated from $Y_k(t=0) = Y_k^o$ to $Y_k(t=\tau^*) = Y_k^*$. It is, of course, also the result when the species mass balance of the homogeneous reactor (transient PSR) is integrated to steady state, as used by Gran (1994), Gran and Magnussen (1996). Then, the mean reaction rate can be expressed as Eq. 3.

Using the argument of De et al. from above on the formulations of Eq. 38 versus Eq. 39, the requirement will be that $\tau^*/(\gamma_\lambda^2\chi)$ should be larger than τ^*. When $\chi \leq 1$, this is satisfied by the trivial requirement that $\gamma_\lambda < 1$.

Indeed, since the fraction γ_λ must be less than unity, there is a low Reynolds number limit of applicability of the original EDC formulation. For instance, Myhrvold (2003) (doctoral student of the author) attempted to develop a modification of γ_λ for low turbulence Reynolds numbers close to a wall. Due to lack of experimental or DNS data at the time, this work was

just indicative for a solution.

The limit found by De et al. (2011) was restricted to the special implementation of EDC in Ansys Fluent, and not a limit of validity for EDC in general. Nevertheless, the Ansys Fluent implementation has been the basis for a number of discussions and suggested modifications, which will be discussed below. Accordingly, these modifications also inherit the restriction.

6 Modified EDC in literature: Changed constants

6.1 Proposals in literature

Several researchers have suggested changes to the model constants, in particular with a background of reforming and of "MILD" combustion, which partly occurs at very low turbulence Reynolds numbers. It seems to be initiated by Rehm et al. (2009), who tried larger values of both C_γ and C_τ. A suggestion of either increasing C_τ to 3.0 or decreasing C_γ to 1.0 was made by De et al. (2011), which has been adopted by some other investigators. Tables 1-2

A number of suggestions are reviewed chronologically in Tables 1-2. Aminian et al. (2012) tried increased values of C_τ, while keeping C_γ near the original value. Graça et al. (2013) compared effects of changes in C_γ and the constant $C_{\varepsilon 2}$ of the k-ε model. Evans et al. (2015) investigated the relative effects of changing C_γ and $C_{\varepsilon 2}$. Some of the suggestions were parameter variations made to investigate the effects of changing one or both constants. Some proposals were apparently based on mistakes, such as Aminian et al. (2012), who calculated C_γ based on a typo, and Wang et al. (2015), who claimed to follow De et al. (2011), but changed both constants and interchanged the numerical values.

All the studies referred in Table 1 were based on use of Ansys Fluent. In that code, EDC was implemented with C_γ and C_τ as two readily tunable parameters, and the suggestions were made in terms of values for these secondary constants.

6.2 Analysis of proposals

Tables 1-2 show the reaction-rate constant C_R (Eq. 11), the ratio of the fine-structure length scale (Eq. 6) to the Kolmogorov scale, L^*/η, the Reynolds number of the fine structures (Eq. 8), the turbulence Reynolds number at which the viscous part accounts for 10% of the dissipation (Eq. 36), and this ratio at $Re_\mathrm{T} = 200$. The Re_T value that gives $\gamma_\lambda = 1$ is shown as well. The latter three quantities depend on C_γ, however not on C_τ.

The changed constants can be discussed in relation to
– the reaction rate, cf. Eq. 11,
– the fine-structure model, cf. Eqs. 6-8 and 10,
– the variation of γ_λ and the EDC factor with Re_T (Sect. 3.3), and
– the dissipation model, which is related to the Re_T dependency, cf. Eq 36.

It is seen that most of the variant suggestions gave values of the numerical factor C_R that were notably different from its original value. Accordingly, the local reaction rate will be considerably affected. This can be seen in relation to γ_λ and the EDC factor, Eq. 29.

Figure 9 shows γ_λ for a selection of suggested C_γ values, while Fig. 10 shows the EDC factor (Sect. 3.3) with $\chi = 1$ as $\gamma_\lambda^2/(1-\gamma_\lambda^3)$ for the same constants. Since the Re_T axes were limited to 500, results for $C_\gamma > 4.7$ were not visible in these graphs. The tables show that the limiting Re_T where γ_λ reaches unity ranges from 0.06 to 1128, when looking apart from the proposals by Rehm et al. (2009). The variations shown are noted with the reservation that the less-than-unity values of χ have an impact as seen from Fig. 8. Figs. 9,10

Figure 11 shows the spreading of fine-structure length and velocity scales compared to Kolmogorov scales for all suggested constants reviewed in Tables 1-2. Parameter variations (i.e. in C_γ) with a constant C_τ can be observed as points on straight lines in the graph. Due to the considerable spreading of the results in Fig. 11a, an excerpt with axis limits (0,8) is shown in Fig. 11b besides the full graph. It was observed that some proposed modifications led to fine structures that were 1–2 orders of magnitude larger than the Kolmogorov scales, whereas one order of magnitude less for others. The associated Reynolds number Re^* ranged over four Fig. 11

orders of magnitude, Tables 1–2.

The Re_T value giving $\gamma_\lambda = 1$ (last column of the tables) also gave an indication on where the fine-structure length scale approaches the integral length. Some proposals implied that this occurs at a very high Reynolds number. This coincided with prediction of very high values of L^*/η.

The dissipation can be expressed from Eq. 34 as described in Sect. 4. Figure 12 shows the viscous part of the dissipation as a fraction of the total dissipation. The graph is similar to Fig. 7, but for a selection of constants from Tables 1-2. Again, considerable variation is seen, from minimal viscous effects at a low Re_T for $C_\gamma = 0.5$, to dominating viscous effects at notably high Re_T for C_γ above 5. Furthermore, it can be shown that for any set of constants, $\varepsilon_2/\varepsilon = 0.43$ for $Re_T = Re^*$. Fig. 12

6.3 Elements of a discussion

A discussion can be made with the presumption that the various suggestions were based on an acceptance of the formal model. This includes the cascade model with dissipation terms and fine-structure scales. Furthermore, EDC is always used in combination with a turbulence model (RANS in the present context, but also for LES). The terms and constants of that model have been calibrated to certain limiting cases. Since turbulence occurs with and without combustion, some elements of the turbulence-chemistry interaction model are also relevant for non-reacting flows.

The turbulence Reynolds number at which viscous modifications of the dissipation should occur, depends on the criteria adopted. From the data presented by Perot and de Bruyn Kops (2006) appeared (cf. Sect. 4) that within Re_T values of 100-200, the effects of viscosity should be visible, while increase with a lower Re_T value. Table 1 shows that the original EDC constants satisfied this, while many of the alternative suggestions engaged the viscous forces at either much lower or much higher values of the Reynolds number.

Nevertheless, the changed constants appeared to improve the results for some specific cases.

It is worth noting that the referred studies were based on Ansys Fluent. As discussed above, Sect. 5.2, Fluent used a batch reactor integrated from the mean value, and $\chi = 1$ was used for all cases. At moderate and low Re_{T}, the mean value inlet reduces the reaction rate, while setting $\chi = 1$ increases it.

From Tables 1-2 was seen that several modifications, including the recommendation of De et al. (2011), reduced the constant C_R, that is, reduced the reaction rate. A relevant question - or hypothesis - is whether the Fluent implementation of EDC created a need of modified constants for highly diluted oxidizer and low turbulence Reynolds numbers.

In some of the referred studies, changes of other constants were tried along with the EDC constants. For instance, Graça et al. (2013) compared results when increasing C_γ and when increasing the constant $C_{\varepsilon 2}$ of the k-ε model. A widely used approach to round jets is to increase $C_{\varepsilon 1}$ of the standard k-ε model. This will increase ε and reduce k and k^2/ε (i.e. turbulence viscosity). This is not done primarily to correct ε, but to reduce the radial spreading of the jet flow. A side effect of increasing ε is reduction of τ^* and increase of γ_λ. The effect is similar to reducing C_τ and increasing C_γ. Alternatively, a $C_{\varepsilon 1}$ increase can partly be compensated by increasing C_τ and reducing C_γ. Similar changes can occur by shifting to another turbulence model.

Furthermore, predictions of ε, either directly or from ω or some other time or length scale quantity, are particularly challenging in inflow zones to a reacting flow, due to modeling as such, to uncertainties in the turbulence conditions of the inflow, to limitations in the numerical resolution etc. These challenges propagate into the combustion model using input from the turbulence predictions. Changes in the combustion model might in some cases act to compensate for deficiencies in the modeling of turbulence.

One criterion for evaluating the proposed constants can be set from the fine-structure region fraction, γ_λ. If the proposal gives a value of γ_λ close to unity for a high turbulence Reynolds number, Re_{T}, the set of constants can be disregarded. A tentative limit can be set by requiring $\gamma_\lambda < 0.75$ for a Re_{T} above, say, 250. This corresponds to unity γ_λ at $Re_{\mathrm{T}} = 80$ or higher. Another criterion, similar to the former, can be a requirement that the ratio of the viscous

term to the total dissipation, $\varepsilon_2/\varepsilon$, is less than, say, 0.5 at $Re_\mathrm{T} > 50$. A low-Re_T limit can, tentatively, be to require $\varepsilon_2/\varepsilon > 0.5$ at $Re_\mathrm{T} < 1$.

The relation to the ratio of turbulence shear stress to turbulence energy may also be considered. Suggestions for a value of $C_{\mathrm{D}1}$ at, say, 0.3 would correspond to a C_μ or β^* of 0.2 in, respectively, the k-ε (Launder and Spalding, 1974) and k-ω (Saffman and Wilcox, 1974, Wilcox, 1988) turbulence models.

The indisputable wide use of EDC indicates that the resulting mean reaction rate is reasonably well modeled. Accordingly, suggested constants that give a value of the constant C_R that differs by an order of magnitude or more from the original model, can be questioned.

Even when considering these criteria with the ample limits sketched here, most of the suggestions would be excluded. A handful of suggestions would remain, which are moderate deviations from the original constants.

7 Some other modifications

7.1 Combined Arrhenius and EDC

Shiehnejadhesar et al. (2014) combined the EDC expression for reaction rate with "finite rate kinetics", that is, an Arrhenius model at low turbulence Reynolds numbers. The two contributions were added with a weighting function. The two terms had equal weight at $Re_\mathrm{T} = 1$. This function was adjusted by Shiehnejadhesar et al. (2015), where the two terms had equal weight at $Re_\mathrm{T} = 3$. They also proposed a near-wall model based on the same idea, where the blending function was based on the dimensionless wall distance.

A concern that can rise here is the use of mean conditions in the Arrhenius expression for a turbulent flow. Moreover, no near-wall or other low Re_T combustion data seemed to be used in the choice and tuning of the weighting functions. Another, more conceptual, concern would be the cascade, which should be very short - or completely collapsed - at the very low Re_T anticipated by this modification. The EDC component of the model seemed just to limit the

EDC factor to unity.

A somewhat related approach was tried by Myhrvold (2003) (p. 97), who proposed to modify γ_λ at low Re_T near walls. This was, at least, more conceptually consistent with EDC. Although some data (2-dimensional DNS) were available and used for validation, the ideas were not pursued due to shortage of near wall combustion data at the time. Moreover, the cascade model still remained to be dealt with.

7.2 Cascade based on fractal theory

An interesting development is the application of fractal theory to model the cascade and the fine structures. A proposal along these lines was made by Farokhi and Birouk (2018a,b). Their model can be expressed as the time scale

$$\tau^* = 0.5\frac{k}{\varepsilon}(\gamma^*)^{\frac{1+\frac{2}{3}-\frac{D_c}{3}}{3-D_c}}, \tag{53}$$

the EDC factor (cf. Sect. 3.3)

$$g_{\mathrm{EDC,FB}} = \frac{\gamma_\lambda^2}{1-\gamma^*} = \frac{(\gamma^*)^{\frac{2}{3}\left(\frac{D_c-2}{3-D_c}\right)}}{1-\gamma^*} \tag{54}$$

and the fine-structure mass fraction

$$\gamma^* = \left(\frac{L^*}{\eta}\right)^{3-D_c}(Re_\mathrm{T}^{-3/4})^{3-D_c}, \tag{55}$$

with the fractal dimension

$$D_c = 1 + \frac{\log(Re_\mathrm{T}^{3/2}/\pi)}{\log(Re_\mathrm{T}^{3/4})}, \quad \text{where} \;\; 2.0 \le D_c \le 2.8. \tag{56}$$

In addition, the fine-structure length scale was adapted as

$$\frac{L^*}{\eta} = \frac{w}{w+Re_\mathrm{T}}1.75 + \frac{Re_\mathrm{T}}{w+Re_\mathrm{T}}3.15, \tag{57}$$

with the weighting parameter tuned to $w = 50$. The latter expression implied a smooth transition of L^*/η from 1.75 at very low Re_T to 3.15 at high Re_T. This can be compared to the original constant value of 1.42.

The fine-structure mass fraction from Eq. 55 reached $\gamma^* = 1$ at $Re_T = 2.0$. It is compared to γ_λ^2 and γ_λ^3 from the original EDC in Fig. 13. The time scale of Eq. 53 is compared to the original time scale expressed from Eq. 11. In the third graph, the EDC factor of Eq. 54 is compared to that of the 1989 version of EDC with $\chi = 1$, and with χ calculated from Eqs. 25–27 with $\lambda = 0.90$ and $c = 0.6$ (also shown in Figs. 4–5). Fig. 13

The major difference observed was in the γ^*, which appeared to be nearly constant and fairly large for most of the Re_T range. Similarly, τ^* was larger than in the original EDC. The difference seems to be less than that imposed by the difference in γ^*. At low Re_T, the EDC factor was reduced with the new model compared to that of $\chi = 1$. However, in this aspect, the effect of the new model seems to be quite similar to including the non-unity χ of the 1989 version. There seemed also to be a difference in the interpretation of the quantity γ_λ between Magnussen and said authors.

7.3 Modified reaction rate model for low Reynolds and Damköhler numbers

These comments will not be complete without mention of the approach persuaded by Parente at al. (2016), Bao (2017) and Evans et al. (2018). They introduced the laminar flame speed and thickness, and thereby the local Damköhler number into the EDC expressions. Furthermore, more dependency on the turbulence Reynolds number was implemented. Since this development was an ongoing activity, it was found premature to include any discussion in the present paper. A comment, though, could be that the development still seems to maintain the multi-step cascade model for relatively low Reynolds numbers.

8 Overall discussion

In the textbook (Ertesvåg, 2000), it was pointed out that one likely reason for the undoubted success of the k-ε model was that some leading groups at an early point of time adopted the model with no or very limited variations. Actually, when studying the origin and history of the model, constants and other modeling choices can be regarded as highly debatable. On this background, it seemed important that the scientific community gathered knowledge about which deviations should be expected for which cases, rather than trying to make ad-hoc adjustments for each case. Similarly, Magnussen has always advocated using models for practical applications, including EDM (1976) and EDC, without changing constants.

The aim of the present study was not to "shoot down" any of the proposed modifications of EDC. However, it seemed apparent that for many of the suggestions, their effects and consequences constitute an unfortunate burden that by itself can make them non-viable.

Several of the proposals were based on a reduced version of EDC, in particular by generally assuming that the fraction of reacting fine structures is unity ($\chi = 1$). Moreover, quite a few proposals were based on the deviating implementation in Ansys Fluent, which in particular have notable effects at low turbulence Reynolds numbers. Moreover, changes were made in the turbulence model, not with the aim of correcting the turbulence quantities, but to modify secondary or tertiary effects of the model (e.g. spreading of a jet). It can be reasonable to ask whether some of the suggested modifications simply compensate for unawareness of the implicit deviations and defects.

9 Concluding remarks

A notable number of modifications for EDC proposed in literature is reviewed. The reacting fraction of fine structures is often neglected by users, in particular since it is not included in the EDC implementation of the most popular commercial code, Ansys Fluent. It is shown that the reacting fraction includes damping of non-stoichiometric and incompletely reacted mixtures and damping at low turbulence Reynolds numbers, which are effects requested in

literature.

The EDC fine structure-reactor implementation of Ansys Fluent includes another deviation from the original EDC, which causes some of the defects claimed on EDC in literature, in particular a Reynolds number limit of validity.

The original EDC constants implicate that viscous effects are inactive at very high turbulence Reynolds numbers and acting at low turbulence Reynolds numbers. This coincide with fine-structure mass fractions that are low at high Reynolds numbers and approaching unity at low Reynolds numbers. Furthermore, the fine-structure length scales predicted are of the order of the Kolmogorov scale. In contrast, some of the proposed modifications have large deviations, such as fine-structure lengths 2-3 orders of magnitude larger than, or one order less than, the Kolmogorov scale. It is shown that reasonable assumptions on effects of high and low Reynolds number disregard many proposals for modifying the EDC constants. The reaction rates of some suggestions are two orders of magnitude less than, some others an order larger than the original EDC.

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Nomenclature

C_{D1},C_{D2}	constants of EDC (-)
C_{R}, C_γ, C_τ	secondary constants of EDC (-)
$C_{\varepsilon 1}$, $C_{\varepsilon 2}$, C_μ	constants of k-ε model (-)
c	extent of reaction (-)
D_c	fractal dimension (-), Eq. 53
g_{EDC}	EDC-factor (-), Eq. 29
F	ratio of mean reaction rates (-), Eq. 42
f	mixture fraction (-)
k	turbulence energy ($\mathrm{m}^2/\mathrm{s}^2$)
L	length scale (m)
$\dot{m}^*$	mass inflow to EDC reactor per reactor mass (-)
n	turbulence energy decay exponent (-)
R	time scale ratio (-), Eq. 50
R_k	volumetric reaction rate of species k ($\mathrm{kg}/(\mathrm{s}\cdot\mathrm{m}^3)$)
Re	Reynolds number (-)
Re_{T}	turbulence Reynolds number, $k^2/(\nu\varepsilon)$ (-)
r	stoichiometric oxidizer requirement of the fuel, mass based (kg/kg)
t	time (s)
T	temperature (K)
u	velocity scale (m/s)
u'	turbulence velocity scale (m/s)
v	Kolmogorov velocity scale (m/s)
w	weighting parameter, Eq. 57 (-)
Y_k	mass fraction of species k (-)

α_H, α_L	constants in the model of Eq. 35 (-)
β^*	constant in Saffman–Wilcox k-ω turbulence model (-)
γ^*	mass of fine structures divided by total mass (-)
γ_λ	mass of fine-structure regions divided by total mass (-)
ε	turbulence energy dissipation rate (m^2/s^3)
η	Kolmogorov length scale (m)
θ	time scale, k/ε (s)
λ	variable of turbulence model, Eq. 35 (m^{-1})
λ	excess air ratio, reciprocal of equivalence ratio (-)
ν	kinematic viscosity (m^2/s)
ρ	mass density (kg/m^3)
τ	time scale (s)
χ	reacting fraction of fine structures (-)
ω	turbulence strain rate or frequency (s^{-1})

Superscripts

$\overline{}$	average
$\sim$	mass-weighted (Favre) average
*	fine-structure (reactor) quantity of EDC
^{o}	surroundings of EDC fine-structure reactor

Subscripts

BaR	batch reactor
fu	fuel
ox	oxidizer
pr	product
st	stoichiometric

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List of Figures

Table 1: Suggested and tried changes of constants in EDC, with effects on reaction-rate constant (Eq. 11), fine-structure scales (Eqs. 6 and 8), viscous term of dissipation ($\varepsilon_2/\varepsilon$, Eq. 36) and the lower limiting turbulence Reynolds number (at $\gamma_\lambda = 1$, Eq. 9)

C_γ	C_τ	C_{D1}	C_{D2}	C_R	L^*/η	Re^*	Re_T at $\varepsilon_2/\varepsilon = 0.10$	$\varepsilon_2/\varepsilon$ at $Re_\mathrm{T} = 200$	Re_T at $\gamma_\lambda = 1$	Ref.
2.130	0.4082	0.135	0.50	11.1	1.42	2.47	222	0.11	20.6	(a)
2.1377	0.4082	0.134	0.50	11.2	1.43	2.49	226	0.11	20.9	(a')
3.2066	0.4082	0.060	0.50	25.2	2.14	5.60	1142	0.32	106	(b)
5.56	0.4082	0.020	0.50	75.7	3.71	16.8	19321	0.67	956	(b,f)
8.45	0.4082	0.0086	0.50	175	5.63	38.9	55062	0.84	5098	(b)
13.0	0.4082	0.0036	0.50	414.	8.67	92.0	308459	0.93	28561	(b)
4.0	8.0	0.750	192	2.0	52.3	171	2765	0.47	256	(b)
5.0	8.0	0.480	192	3.1	65.3	267	6750	0.62	625	(b)
6.0	8.0	0.333	192	4.5	78.4	384	13997	0.71	1296	(b)
7.0	8.0	0.245	192	6.1	91.4	523	25931	0.78	2401	(b)
10.0	8.0	0.120	192	12.5	131	1067	108000	0.88	10000	(b)
13.0	8.0	0.071	192	21.1	170	1803	308459	0.93	28561	(b)
1.9239	0.4082	0.165	0.50	9.1	1.28	2.01	148	0.078	13.7	(c)
2.3515	0.4082	0.111	0.50	13.6	1.57	3.01	330	0.15	30.6	(c)
2.1377	3.0	0.985	27.0	1.52	10.5	18.2	226	0.11	20.9	(c,g)
1.0	0.4082	0.612	0.50	2.45	0.67	0.54	10.8	0.0066	1.0	(c,g,j)
2.1637	0.4082	0.131	0.50	11.5	1.44	2.55	237	0.12	21.9	(d)
2.1637	1.5	0.481	6.75	3.12	5.30	9.34	237	0.12	21.9	(d)
2.1637	3.	0.961	27.0	1.56	10.6	18.7	237	0.12	21.9	(d)
5.0	0.4082	0.0245	0.50	61.2	3.33	13.6	6750	0.62	625	(e)
3.20	0.4082	0.0598	0.50	25.1	2.13	5.57	1132	0.32	105	(f)
4.40	0.4082	0.0316	0.50	47.4	2.93	10.5	4048	0.54	375	(f)
0.5	0.4082	2.45	0.50	0.61	0.33	0.14	0.675	0.00042	0.063	(g)
0.75	0.4082	1.09	0.50	1.38	0.50	0.31	3.4	0.0021	0.32	(g)
1.5	0.4082	0.272	0.50	5.5	1.0	1.22	55	0.032	5.1	(g)
2.5	0.4082	0.098	0.50	15.3	1.67	3.40	422	0.18	39.1	(g)
0.5	3.0	18.0	27.0	0.083	2.45	1.0	0.68	0.00042	0.063	(g)
0.75	3.0	8.0	27.0	0.19	3.67	2.25	3.4	0.0021	0.32	(g)
1.0	3.0	4.5	27.0	0.33	4.90	4.0	10.8	0.0066	1.0	(g)
1.5	3.0	2.0	27.0	0.75	7.35	9.0	54.7	0.032	5.6	(g)
2.5	3.0	0.720	27.0	2.1	12.2	25.0	422	0.18	39.1	(g)
3.0	1.0	0.167	3.0	4.6	4.90	12.0	875	0.28	81.0	(h)
1.8	1.0	0.463	3.0	3.2	2.94	4.32	113	0.062	10.5	(i)
1.8	1.5	0.694	6.75	2.2	4.41	6.48	113	0.062	10.5	(i)
2.1377	1.0	0.328	3.0	4.6	3.49	6.09	226	0.11	20.9	(i)
2.1377	1.5	0.492	6.75	3.0	5.24	9.14	226	0.11	20.9	(i)
2.46	1.0	0.248	3.0	6.1	4.02	8.07	396	0.17	36.6	(i)
2.46	1.5	0.372	6.75	4.0	6.03	12.1	396	0.17	36.6	(i)
1.12	1.0	1.20	3.0	1.3	1.83	1.67	17.0	0.010	1.57	(i)
1.12	1.5	1.79	6.75	0.84	2.74	2.51	17.0	0.010	1.57	(i)
2.46	0.4082	0.101	0.50	14.8	1.64	3.29	396	0.17	36.6	(i)
1.75	5.62	2.75	94.8	0.54	16.1	23.0	101	0.056	9.4	(j)
2.37	5.62	1.50	94.8	1.0	21.8	42.1	341	0.15	31.5	(j)

References: (a): original, Magnussen (1981), Ertesvåg and Magnussen (2000), (a'): variant of original, (b): Rehm et al. (2009), (c): De et al. (2011), (d): Aminian et al. (2012), (e): Graça et al. (2013), (f): Xu et al. (2014), (g): Evans et al. (2015), (h): Wang et al. (2015), (i,j): Farokhi and Birouk (2016a,b),

Table 2: Suggested and tried changes of constants in EDC, with effects on reaction-rate constant (Eq. 11), fine-structure scales (Eqs. 6 and 8), viscous term of dissipation ($\varepsilon_2/\varepsilon$, Eq. 36) and the lower limiting turbulence Reynolds number (at $\gamma_\lambda = 1$, Eq. 9)

C_γ	C_τ	C_{D1}	C_{D2}	C_R	L^*/η	Re^*	Re_T at $\varepsilon_2/\varepsilon = 0.10$	$\varepsilon_2/\varepsilon$ at $Re_\mathrm{T} = 200$	Re_T at $\gamma_\lambda = 1$	Ref.
2.130	0.4082	0.135	0.50	11.1	1.42	2.47	222	0.11	20.6	(a)
1.96	0.4082	0.159	0.50	9.4	1.31	2.09	159	0.083	14.8	(k)
1.07	0.4082	0.535	0.50	2.8	0.71	0.62	14.2	0.0086	1.3	(k)
1.47	1.90	1.32	10.8	1.14	4.56	5.47	50	0.029	4.7	(k)
1.00	2.14	3.21	13.7	0.47	3.50	2.85	10.8	0.0066	1.0	(k)
0.82	2.14	4.77	13.7	0.31	2.87	1.92	4.9	0.0030	0.5	(k)
1.25	1.78	1.71	9.51	0.88	3.64	3.71	26	0.016	2.4	(k)
1.77	2.00	0.958	12.0	1.57	5.78	8.35	106	0.058	9.8	(k)
1.798	0.2896	0.134	0.25	11.2	0.85	1.24	113	0.061	10.4	(l)
1.00	0.0893	0.134	0.0239	11.2	0.15	0.12	10.8	0.0066	1.0	(l)
2.542	0.5773	0.134	1.0	11.2	2.40	4.98	451	0.19	41.8	(l)
5.795	3.0	0.134	27	11.2	28.4	134	12180	0.70	1128	(l)
1.9	1.47	0.611	6.48	2.46	4.56	7.08	141	0.074	13.0	(m)
1.5	1.47	0.98	6.48	1.53	3.60	4.41	55	0.032	5.1	(m)

References: (a): original, (k): Parente et al. (2016), (l): Mardani (2017), (m): Li et al. (2017)

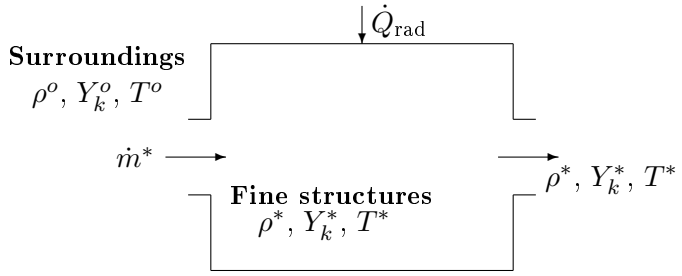

Figure 1: Schematical fine-structure reactor

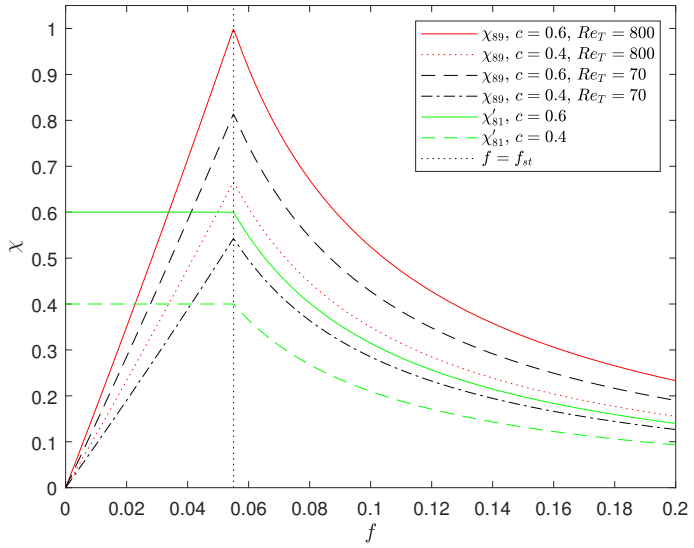

Figure 2: χ (or $\chi\eta'$) of the 1989 version and χ' of the 1981 version as functions of mixture fraction f at specified values of extent of reaction c and Re_{T}. The vertical line shows the stoichiometric mixture.

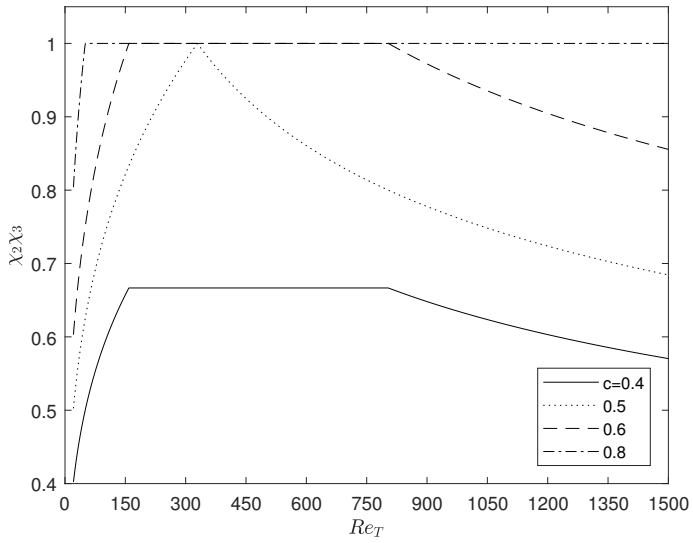

Figure 3: The product $\chi_2\chi_3$ of the 1989 version as a function of the turbulence Reynolds number Re_T for specified c values

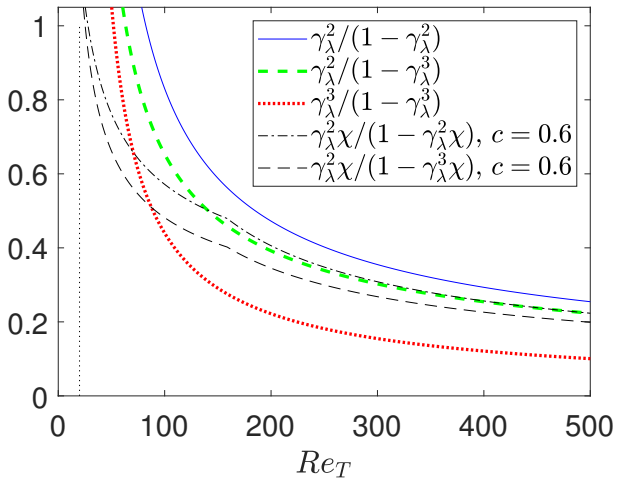

Figure 4: Comparison of the different factors for the mean reaction rate with and without χ of 1989. The excess air ratio was set to $\lambda = 0.9$.

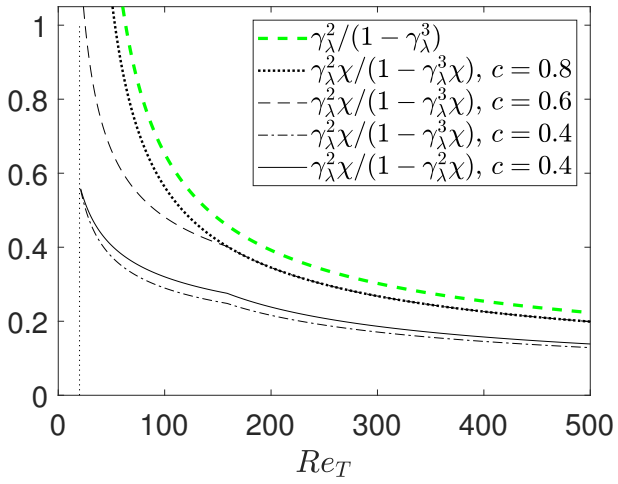

Figure 5: Comparison of the factor for the mean reaction rate with χ of 1989 and varied c. The excess air ratio was set to $\lambda = 0.9$.

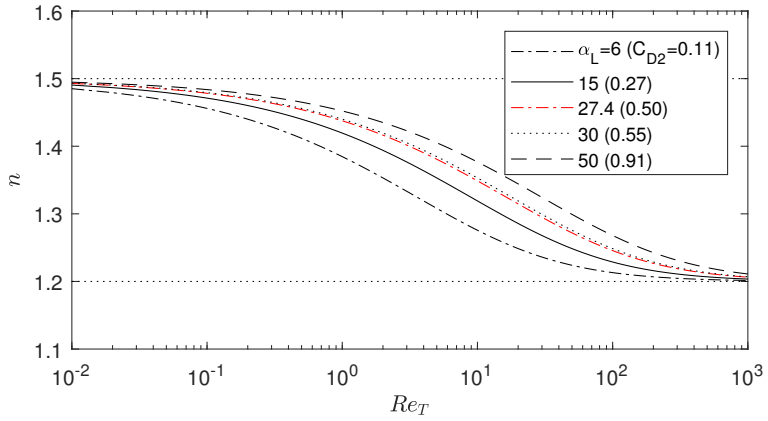

Figure 6: Decaying turbulence, κ^2 low wavenumber spectrum, power law exponent from the two models, Eq. 35 and Eq. 34, with different values of constants α_L or C_{D2} (with $\alpha_H = 1$ or $C_{\mathrm{D1}} = 0.135$).

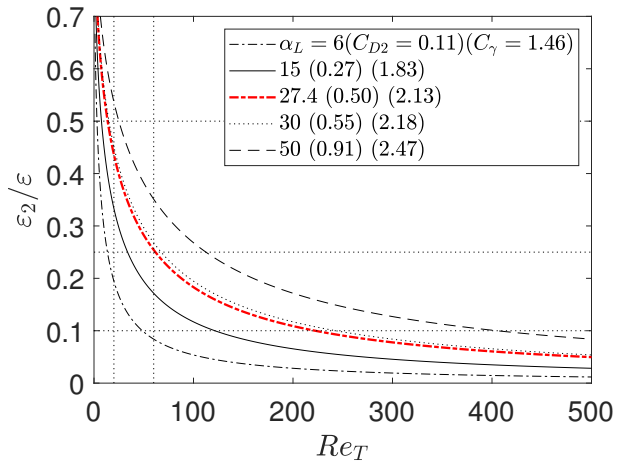

Figure 7: Ratio of the viscous dissipation term to the total dissipation, Eq. 35 or Eq. 34, with different values of constants α_L or C_{D2} (with $\alpha_H = 1$ or $C_{\mathrm{D1}} = 0.135$). The dotted vertical lines show Re_{T} of 20 and 60.

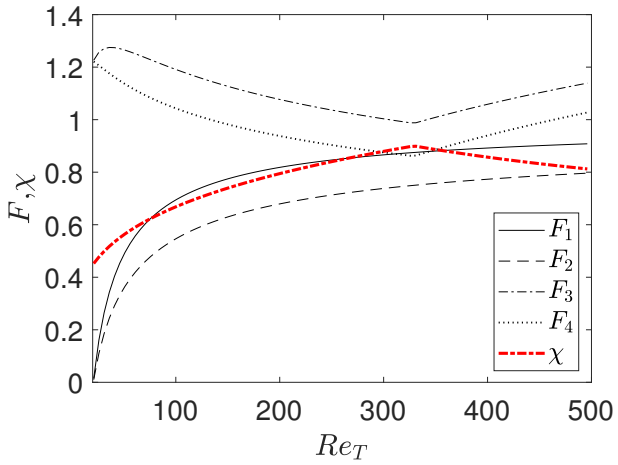

Figure 8: Ratio of the mean reaction rates of the Fluent BaR/PFR implementation to some variants of the original model. χ was evaluated for $\lambda = 0.90$, $c = 0.50$.

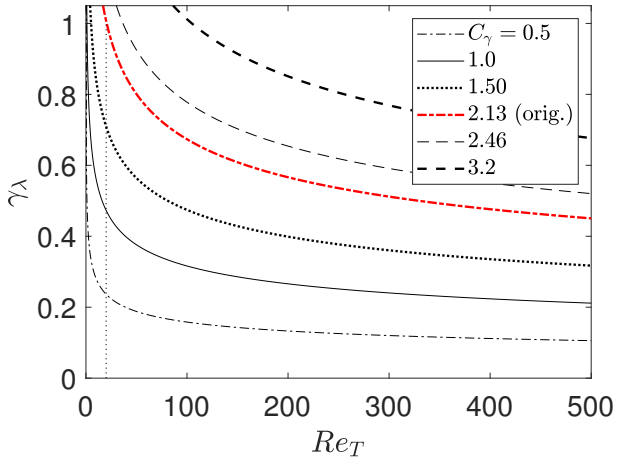

Figure 9: γ_λ as a function of Re_T for a selection of suggested modified constants. The dotted vertical line shows $Re_\mathrm{T} = 20$.

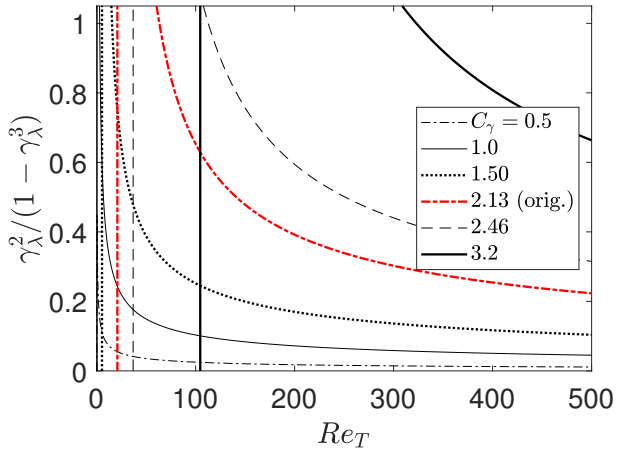

Figure 10: The EDC factor $\gamma_\lambda^2\chi/(1-\gamma^3\chi)$ as a function of Re_T with $\chi = 1$ for a selection of suggested modified constants. The vertical lines denote where γ_λ reaches unity.

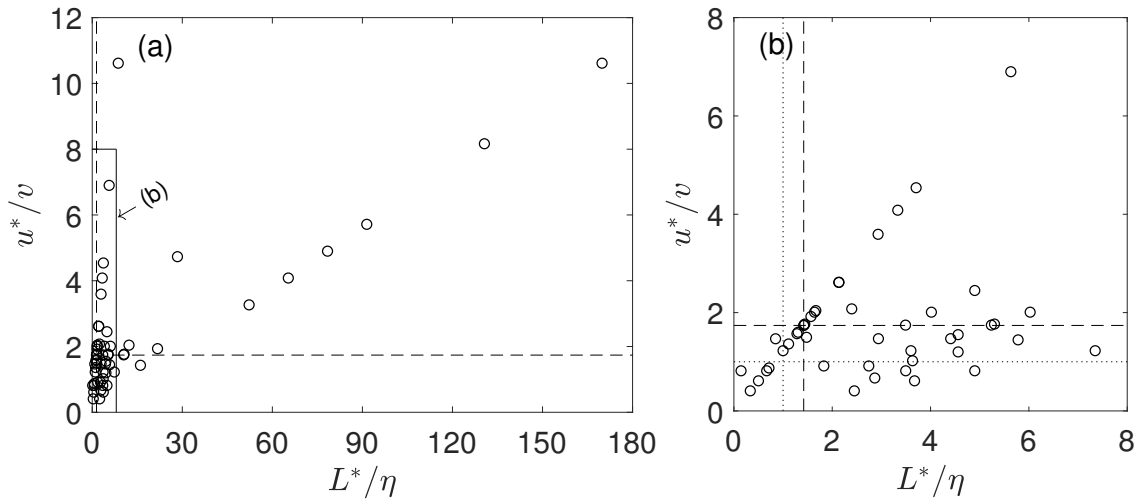

Figure 11: Combined values of fine-structure length and velocity scales normalized to the Kolmogorov scales for all suggestions listed in Tables 1-2. The values of the original model is shown by the dashed lines and Kolmogorov scales with dotted lines. The solid lines in Fig. a denote the extract shown in Fig. b.

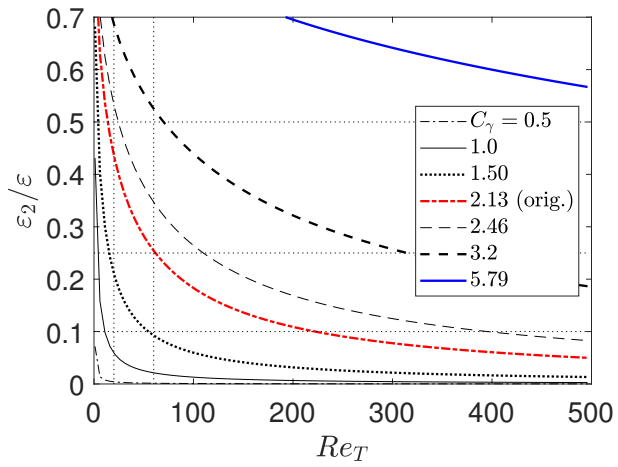

Figure 12: Ratio of the viscous dissipation term to the total dissipation, Eq. 35 or Eq. 34, for a selection of suggested modified constants. The dotted vertical lines show Re_T of 20 and 60.

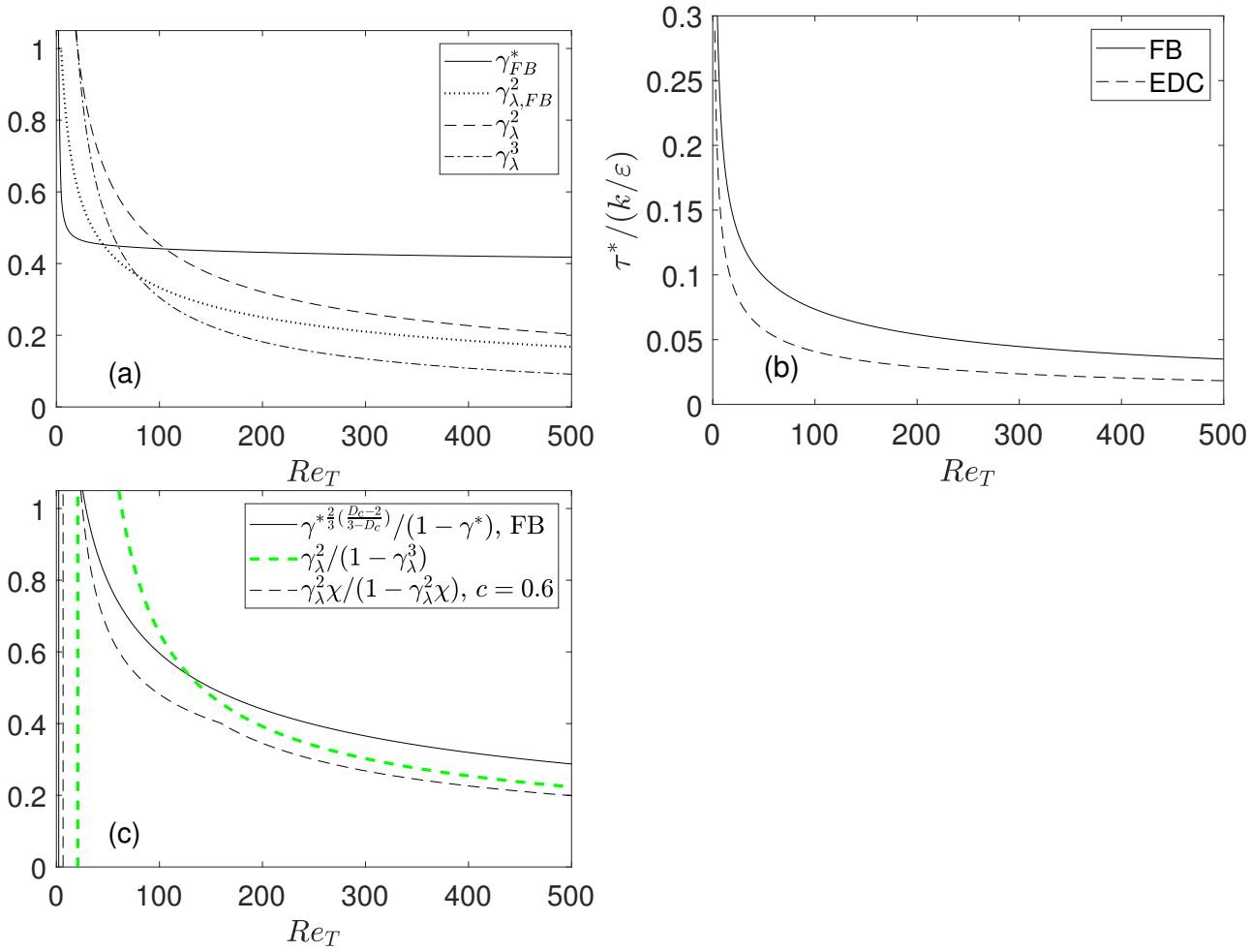

Figure 13: The fine-structure mass fraction (a) and timescale (b), and the EDC factor (c) for the model of Farokhi and Birouk (2018a,b) ("FB") compared to variants of the original EDC. When calculating χ (1989 version), the excess air ratio was set to $\lambda = 0.9$ and the extent of reaction to $c = 0.6$.