

EMISSION PREDICTIONS IN DIESEL ENGINES USING A NON-EQUILIBRIUM TURBULENCE DISSIPATION CORRECTION FOR THE k - ε MODEL

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ABSTRACT

A correction for the turbulence dissipation rate, based on non-equilibrium turbulence considerations from rapid distortion theory, has been derived and implemented in combination with the *RNG* $k - \varepsilon$ model in a *KIVA*-based code. This correction reflects the time delay between changes in the turbulent kinetic energy due to changes in the mean flow and its turbulence dissipation rate, and it is shown that this time delay is controlled by the turbulence Reynolds number. Combustion simulations of two heavy-duty DI diesel engines have been performed using the *RNG* $k - \varepsilon$ model with and without the dissipation rate correction. The focus of these computations has been on the nitric oxide formation and the net soot production. These simulations have been compared with experimental data and their predictions are explained in terms of the turbulence dissipation effect on the transport coefficients for mass and heat diffusion. It has been found, that the dissipation correction yields consistent results with observations reported in previous studies.

INTRODUCTION

The characteristic time combustion model of Abraham et al. [1], as adapted to diesel combustion by Kong et al. [2], requires adjustments to the combustion rates in order to match the experimental cylinder pressures for different engines. The need for these adjustments can be explained in terms of non-equilibrium turbulence, as has been demonstrated in a study by Tanner et al. [3]. In fact, due to piston movement and especially the fuel injection process, the flows in DI diesel engines are transient in nature and therefore, the equilibrium turbulence assumption that turbulence production balances its dissipation at any instant, is violated. Consequently, turbulence predictions based on the two equation k - ε -type turbulence models, where the turbulence equilibrium assumption is violated, are inaccurate.

Various approaches have been investigated by numerous researchers in order to remedy the shortcomings of the linear k - ε -based turbulence models. Improvements of this model, based on the theory of re-normalization groups (RNG), have been achieved by Yakhot et al. [4] and successfully introduced to spray combustion simulations by Han et al. [5]. However, uncertainties in the dissipation transport equation still remain and have been investigated in a recent study by Bianchi et al. [6]. In this investigation, the change of the

molecular viscosity, predicted by the rapid distortion theory, have been integrated into the ε -equation. This is a further development of a study by Coleman and Mansour [7], where an additional closure relation has been developed to account for rapid distortion effects.

In the present study, the delay between the turbulence kinetic energy and its dissipation rate in transient flows is modeled by imposing an additional constraint on the dissipation rate. This dissipation rate correction (ε -correction) considers the local change of the turbulence Reynolds number and directly influences the turbulence viscosity. This ε -correction has previously been validated by means of experimental turbulence length scales measured in a small experimental *Lombardini* engine operating in motored mode [8, 9]. In addition, the effect of this ε -correction on the turbulence length and time scales as well as on the performance of the characteristic time combustion model has been investigated for two heavy-duty DI diesel engines, the *Caterpillar 3406* (CAT) and the *Sulzer S20* (S20).

The focus of the present study is on the influence of this ε -correction on the pollution predictions of the two engines. Particular attention has been given to the influence of this ε -correction on the soot and nitric oxide formation for various operating conditions. The effect of the ε -correction is discussed in view of the turbulence viscosity and its effect on the transport coefficients for the heat conduction and the species diffusion.

EQUILIBRIUM AND NON-EQUILIBRIUM TURBULENCE

The equilibrium hypothesis, which states that the instantaneous turbulence production rate equals the turbulence dissipation rate, is one of the fundamental assumptions in eddy viscosity-based turbulence modeling. If only one length scale is used to characterize turbulence, say the macro length scale L_ε , as is the case in the 2-equation k - ε model, then L_ε represents all the length scales of the turbulence, and the turbulence can be described as being in equilibrium. In this case, the turbulence is self-similar since all scales adjust to flow changes at the same rate.

Based on the equilibrium hypothesis, the (mass specific) dissipation rate, ε_{eq} , can be expressed as $\varepsilon_{eq} \propto q^3/L_I$, where $q = \sqrt{2k/3}$ is the turbulence intensity, k the (mass specific) turbulence kinetic energy and L_I denotes the integral length

scale. For equilibrium turbulence it is assumed that $L_I \propto L_\varepsilon$ which yields the relation

$$\varepsilon_{eq} = C_\varepsilon k^{3/2} / L_\varepsilon \quad (1)$$

where C_ε is a constant.

For highly transient flows, however, the equilibrium turbulence assumption is likely to be violated, and Eq. (1) does not hold. In fact, the energy dissipation cascade adjusts to changes in the mean flow with some delay and different length scales adjust at different rates. Therefore, a non-equilibrium formulation for the turbulence dissipation is required.

Based on the assumption of isotropic compressed turbulence, using elements of rapid distortion theory, Reynolds [10] hypothesized that the Taylor length scale, L_λ , and the integral length scale, L_I , remain proportional to each other during a rapidly distorting flow. Wu et al. [11] has reached the same conclusion based on his direct Navier-Stokes computations applied to rapid compression flows, and a similar conclusion has been reached by Dinsdale et al. [12] in engine measurements. Using this fact, i.e. $L_I \propto L_\lambda$, Han et al. [13] derived the relation $L_\varepsilon \propto Re_t L_I$, where $Re_t = qL_I/\nu_o$ is the turbulent Reynolds number.

Now, based on the fact that $L_I \propto L_\lambda$, Tanner et al. [8] obtained the following relation between the equilibrium and non-equilibrium dissipation rates

$$\varepsilon \propto \varepsilon_{eq} / Re_t \quad (2)$$

Eq. (2) is the key in the interpretation of the time delay between a change in the turbulence kinetic energy, k , and its dissipation rate ε . A change in the mean flow results in an immediate change in k , whereas the turbulence dissipation, which takes place on the smallest length scale, occurs with some delay. In fact, this delay lies in the order of one eddy turn-over time given by $\tau_\varepsilon = L_I/q$. The relation between this time delay and the turbulence Reynolds number is given by the time scale ratio

$$Re_t = qL_I/\nu_o = \tau_m/\tau_\varepsilon \quad (3)$$

where $\tau_m = L_I^2/\nu_o$ is the molecular diffusion time scale, which is independent of the turbulence behavior. According to Eq. (3), a change in the eddy turn-over time τ_ε results directly in a change of Re_t and consequently, Eq. (2) is the statement that the delay in the dissipation rate is controlled by the turbulence Reynolds number.

Influence on the Transport Coefficients and Re_t

In eddy viscosity-based turbulence models, the turbulence viscosity, ν_t is obtained from a dimensional argument as $\nu_t = c_\mu k^2/\varepsilon$, where the constant $c_\mu=0.09$. The (turbulence) heat conduction (heat diffusion) coefficient, K , and the (turbulence) mass diffusion coefficient, D , are determined by the turbulence viscosity via

$$K = \rho\nu c_p / Pr \quad (4)$$

$$D = \nu / Sc \quad (5)$$

Table 1. Specifications for the simulated engines.

	<i>Caterpillar 3406</i>	<i>Sulzer S20</i>
Bore [mm] × stroke [mm]	137 × 165	200 × 300
Engine speed [rev/min]	1600	1000
Orifices × diameter [mm]	6 × 0.259	12 × 0.285
Cells at TDC:		
rad. × azym. × height	24 × 30 × 14	23 × 13 × 14

where ρ is the gas density, $\nu = \nu_o + \nu_t$ is the total viscosity, $\nu_o (\ll \nu_t)$ is the molecular viscosity, c_p is the specific heat at constant pressure and Pr and Sc represent the Prandtl and Schmidt numbers, respectively. Therefore, from these relations it is apparent that a change in the turbulence viscosity leads to proportional changes in K and D .

It follows, that an increase in the mass diffusion leads to an increased mixing between the species, which, in a mixing controlled combustion, leads to an increased rate of heat release and consequently to higher (local) temperatures. In contrast, an increase in the heat conduction coefficient, K , leads to an improved local heat diffusion, and results in a reduction of the local temperatures and hence, counteracts the higher temperatures caused by the increased mixing. Therefore, it is not at all clear that an increased turbulence viscosity leads to higher local temperatures (and, therefore, to higher nitric oxide formations). The net effect of an increased turbulence viscosity will depend on the specific situation at hand. If, for instance, there is another limiting factor for the mixing (e.g. the gas is already fully mixed), then an increase in D will have little effect on the combustion rate and therefore, only the heat diffusion will be increased, which leads to lower local temperatures. On the other hand, if the local heat transport in the reaction zone is dominated by other means than the heat diffusion coefficient (e.g. near a boundary), then an increase in ν_t will primarily result in an increased mixing, hence in an increased heat release and consequently, in higher local temperatures.

Finally, as shown in [8], the turbulence Reynolds number, $Re_t = qL_I/\nu_o$, can be expressed in terms of the local variables ν_t and ν_o by

$$Re_t \propto \sqrt{\nu_t/\nu_o}. \quad (6)$$

Note that this expression is different from the one obtained under the assumption of equilibrium turbulence, where, $Re_t \propto \nu_t/\nu_o$.

EXPERIMENTAL AND COMPUTATIONAL DETAILS

The CAT engine is a single-cylinder research engine, modified from the production version to accommodate the various measurement devices. This engine has been extensively researched during the past decade and the methods used and the results obtained have been reported in numer-

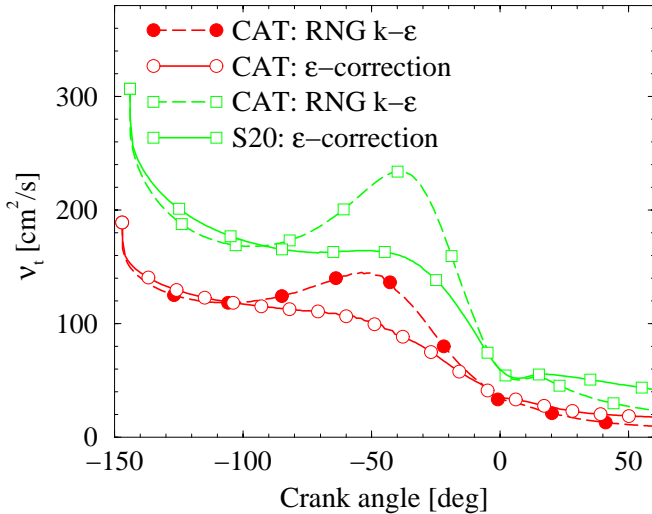


Figure 1. Turbulence viscosity of the *Caterpillar 3406* at high load and the *Sulzer S20* at full load for computations obtained with and without the dissipation correction.

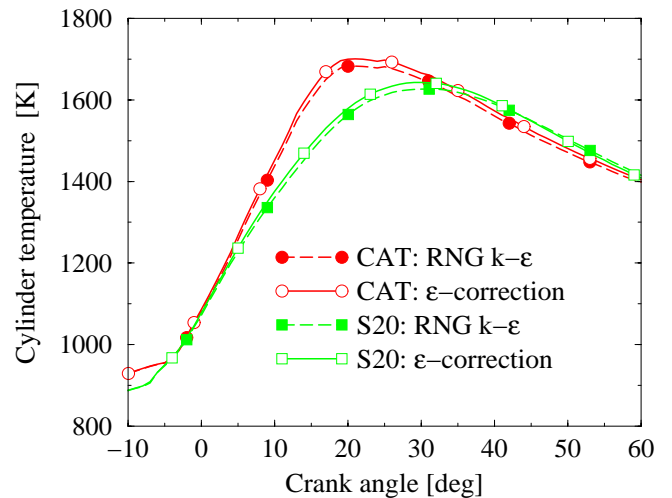


Figure 2. Cylinder temperature of the *Caterpillar 3406* at high load and the *Sulzer S20* at full load for computations obtained with and without the dissipation correction.

ous publications (e.g. [14]). Some of the engine specifications are listed in Table 1.

The experimental data from the S20 engine have been obtained from a nine-cylinder production engine and are reported in [15]. The nitric oxides have been measured by the principle of chemical illumination and then converted into mass specific units. The soot has been determined with a Bosch smoke meter in terms of Bosch smoke units (BSU). In order to permit comparisons with the mass specific units obtained from the simulations, the experimental soot data have been scaled by a factor of 27 to match the simulated values of the standard S20 computations obtained with the *RNG k-ε* model.

Validations of the ε -correction have been performed by means of experimental turbulence length scale measurements in a modified *Lombardini* diesel engine operated in motored mode. These findings are reported in [9].

The computations presented in this study have been performed with an enhanced version of the *KIVA* code [16]. This code is equipped with many new or improved models whose details and/or additional references are given in [9]. The chemical heat release is described by means of the characteristic time combustion model [1, 2] and the nitric oxide formation is modeled by the extended Zeldovich mechanism together with an equilibrium reaction for the hydrogen radicals (c.f. [17]). The soot formation is based on the soot production-oxidation model of Hiroyasu et al. [18] but utilizing the soot oxidation rate of Nagle et al. [19]. The employed turbulence model is the *RNG k-ε* turbulence model as implemented by Han and Reitz [5], together with Eq. (2) which accounts for the ε -correction due to the non-equilibrium turbulence effects, as discussed in the previous section.

The focus of the present investigation has been on the soot and nitric oxide formation for different operating conditions. The CAT simulations have been performed at 75% full load (high load case) and at 25% full load (low load

case). The S20 computations have been carried out at 100%, 75% and 50% of the full load. In addition, different injection timings have been investigated for both engines to illustrate the consistency of the ε -correction for the soot- NO_x trade-off.

For the combustion computations without the ε -correction, the coefficient of the turbulence characteristic time, C_M , had to be adjusted in order to match the experimental cylinder peak pressure. These values were found to be $C_M = 0.25$ for the CAT and $C_M = 2.0$ for the S20. In the corresponding computations with the dissipation correction, these values of C_M have been kept the same for both engines.

RESULTS AND DISCUSSION

The problem of sufficient spatial resolution in the simulation of spray-combustion using the discrete droplet model approach, as is the case in this study, has been addressed in a previous paper [8]. In fact, the choice of the mesh resolution has been a compromise between CPU time and accuracy, where the latter has been measured in terms of the relevant quantities under investigation, the average cylinder pressure and the average turbulence time and length scales. It has been found that the mesh resolution employed in these investigations is adequate and therefore, the same mesh resolutions have been used in the present study.

Soot and NO_x Formation

The turbulence viscosity, ν_t , for the CAT and the S20, computed with and without the ε -correction, are shown in Fig. 1. Both engines show the same behavior: In the compression phase the ε -correction shows a flatter trend in comparison with the standard *RNG k-ε* model, whereas during the combustion phase, the turbulence viscosity of the ε -correction shows higher values. By virtue of Eqs. (4)

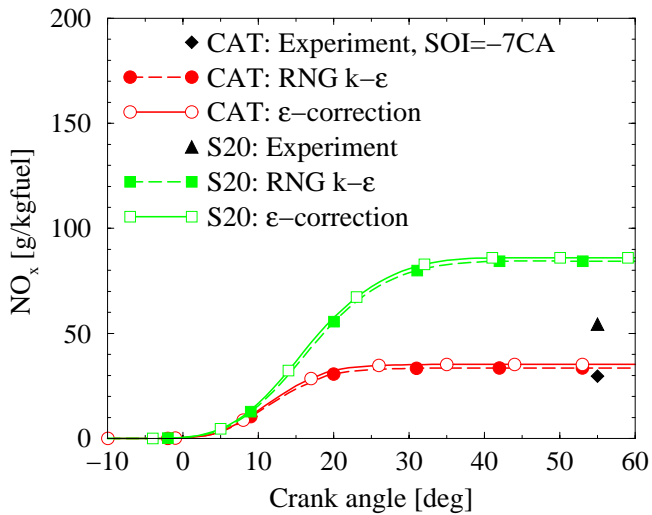


Figure 3. Nitric oxide of the *Caterpillar 3406* at high load and the *Sulzer S20* at full load for computations obtained with and without the dissipation correction.

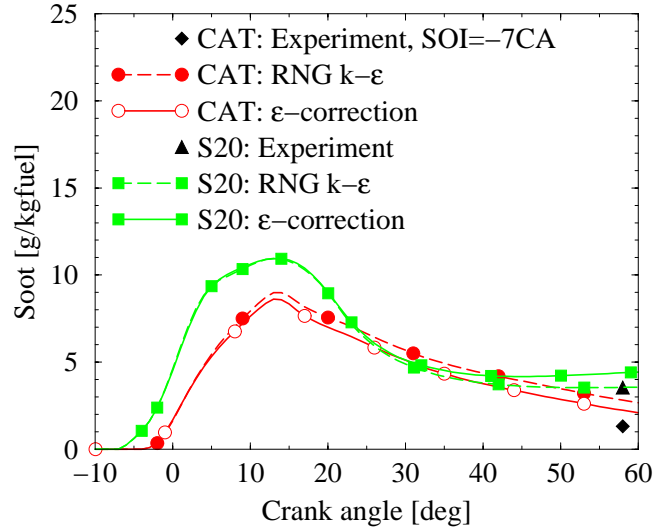


Figure 4. Soot values of the *Caterpillar 3406* at high load and the *Sulzer S20* at full load for computations obtained with and without the dissipation correction.

and (5) the transport coefficient for the heat conduction, K , and mass diffusion, D , behave accordingly. Therefore, during the combustion phase an increase of K (relative to the $RNG k - \epsilon$ prediction) leads to an increase in the local heat diffusion, which results in the decrease of the local temperature. On the other hand, the increase in D results in an improved mixing of the fuel and air, which leads to an increase in the reaction rate, hence an increase in the heat release and therefore, results in higher local temperatures. Consequently, these opposing effects on the local temperature tend to neutralize the nitric oxide production, provided the heat conduction or the mass diffusion are not limited by other means. Therefore, the net effect on the nitric oxide formation due to an increased turbulence viscosity will depend on the particular flow.

As is shown in Fig. 2 for the CAT high load case, the ϵ -correction results in a higher cylinder temperature throughout the combustion phase, which explains the higher NO_x formation shown in Fig. 3. This suggests that the net effect of the heat and the mass diffusions is dominated by the latter, which results in the higher cylinder temperature. On the other hand, the higher cylinder temperatures of the CAT lead to an increased soot oxidation which results in a decrease of the net soot production. This behavior is illustrated in Fig. 4.

The S20 at full load shows a different temperature behavior than the CAT, as is seen in Fig. 2. The cylinder temperature of the ϵ -correction lies above the one obtained by means of the $RNG k - \epsilon$ model only until approximately 40 CA after TDC. After 40 CA the ϵ -correction temperature falls below the one computed with the $RNG k - \epsilon$ model. Consequently, because the maximum NO_x level is already reached at 40 CA, the nitric oxide production is slightly increased, as is illustrated in Fig. 3. The relative decrease in the cylinder temperature of the ϵ -correction after 40 CA results in a decrease of the soot oxidation, hence an increase

in the net soot formation, as is seen in Fig. 4.

For the S20, it appears that the counteracting effects on the local temperature by the increased heat conduction and mass diffusion coefficients are approximately in balance, i.e. the NO_x formation is almost unchanged by the combined effects of the increased heat and mass diffusions. After the injected fuel has been burned, an increase in the mass diffusion coefficient cannot increase the local temperature any further (there is no fuel left), while the increase in K continues to enhance the local heat diffusion. Consequently, the hot spots in the cylinder cool down and the soot oxidation is reduced accordingly, which results in the observed higher soot formation. This mechanism also explains the relative drop of the cylinder temperature of the ϵ -correction case after 40 CA observed in Fig. 2.

The black dots in Figs. 3–4 are measured values and are shown for reference purposes only. It should be remarked that the pollution models, as utilized in this study, have been tuned to the performance of the $RNG k - \epsilon$ model, and therefore, the predictive capability of the ϵ -correction is not fully reflected by the presented data.

The soot- NO_x trade-off for the CAT high load and the S20 full load cases for various injection timings are shown in Figs. 5–6, respectively. For the CAT, the ϵ -correction yields a higher NO_x value and lower soot concentrations in all cases. For the S20, the ϵ -correction leads to a lower net soot production for all injection timings. Except for the standard case with start of injection at -12.5 CA, the nitric oxide values are slightly decreased in comparison with the $RNG k - \epsilon$ computations.

The soot- NO_x trade-off for the CAT low load is shown in Fig. 7 for various injection timing. Both, the ϵ -correction and the $RNG k - \epsilon$ model are capable of predicting the horse shoe shape of the experimental soot- NO_x trade-off curve. The soot and the NO_x predictions are almost identical for all injection timings. This suggests, that the effects of the

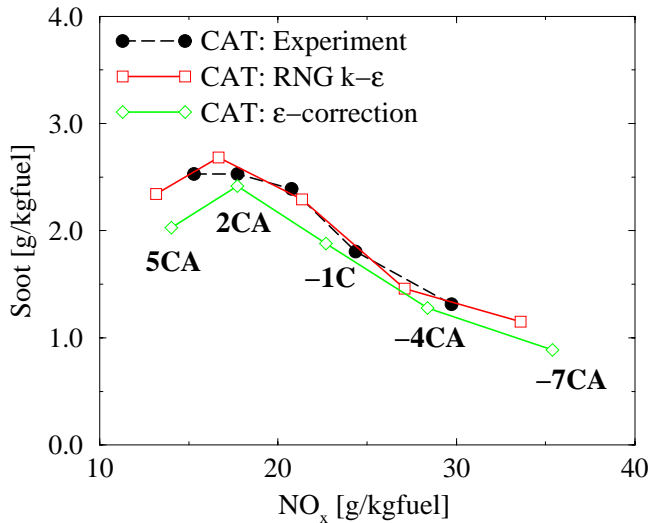


Figure 5. Soot- NO_x trade-off of the *Caterpillar 3406* at high load for various injection timings. The computational data have been obtained with and without the dissipation correction.

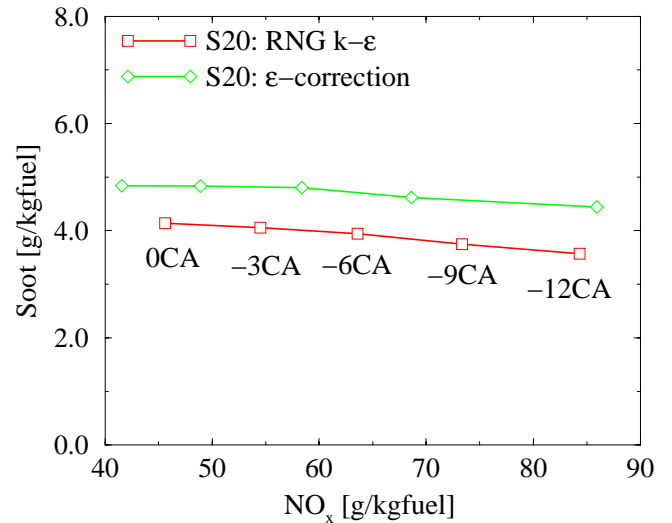


Figure 6. Soot- NO_x trade-off of the *Sulzer S20* at full load for various injection timings. The computational data have been obtained with and without the dissipation correction.

ε -correction on the pollution formation via the transport coefficients D and K are neutralized by each other, as has been discussed above.

Finally, the soot- NO_x trade-off behavior for the S20 at full load and 75% and 50% partial load are shown in Fig. 8. As in the full load cases, the ε -correction predicts higher soot values and slightly higher NO_x concentrations, which are in better agreement with the experimental data. These improved predictions can again be explained in terms of the opposing effects of the transport coefficients K and D on the local gas temperatures, which for the S20, are independent of the engine operating condition.

SUMMARY AND CONCLUSIONS

A correction for the turbulence dissipation rate, based on non-equilibrium turbulence considerations from rapid distortion theory, has been derived and implemented in combination with the $RNG k - \varepsilon$ turbulence model in a $KIVA$ -based code. In particular, the turbulence dissipation rate has been adjusted via the turbulence Reynolds number by $\varepsilon \propto Re_t^{-1} \varepsilon_{eq}$.

Combustion computations have been performed for two heavy-duty DI diesel engines with a focus on the emission prediction capability of the ε -correction. In particular, the influence of the ε -correction on the transport coefficients for mixing and heat conduction has been studied. The ε -correction lead to an improved mixing which resulted in an increased heat release and consequently, in higher local temperatures. Therefore, the production of thermal NO_x has been increased. On the other hand, the ε -correction has lead to an increase in the local heat conduction which, in general, lead to a reduction in the local temperatures and thus opposed the nitric oxide formation. The two phenomena can neutralize the NO_x production, as is almost the case for the S20, or, if the limiting process is the local heat transfer, as in the CAT high load cases, the improved

mixing can lead to an increased nitric oxide formation.

These observations are consistent with the net soot production of the two engines. The increased mixing in case of the CAT has lead to an increase in the soot oxidation and hence resulted in a reduction in the net soot formation. For the S20, the increased local heat dispersion in the very late combustion phase has lead to a decrease in the local temperature and hence a decrease in the soot oxidation, and finally, has resulted in an increase of the net soot production.

The soot- NO_x trade-offs for the CAT and the S20 have been qualitatively well reproduced by the ε -correction. The increased NO_x and the decreased soot predictions for the CAT have been consistent for the injection timing variations at high load. A corresponding statement holds for the S20 injection timing variations at full load.

For the CAT low load cases, however, the effect of the ε -correction is almost not detectable which can be attributed to the opposing effects of the local mass and heat diffusions on the pollution formation. Also, the S20 75% and 50% partial load computations with the ε -correction showed the same trend as in the full load cases. Further, a slightly improved soot- NO_x trade-off behavior has been observed over the ones of the $RNG k - \varepsilon$ computations.

ACKNOWLEDGMENT

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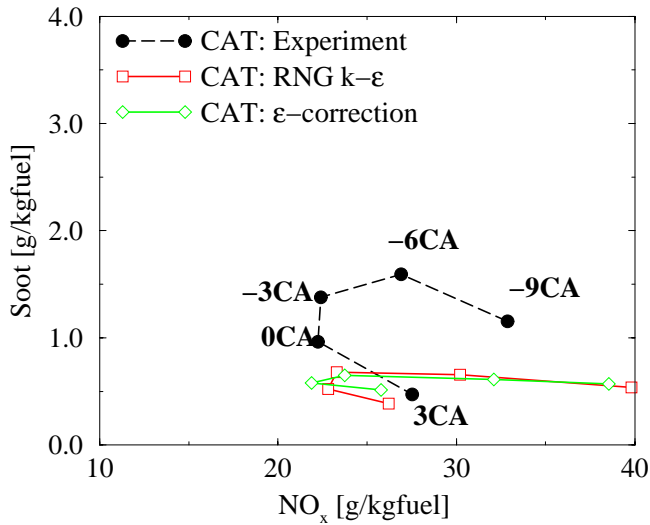


Figure 7. Soot- NO_x trade-off of the *Caterpillar 3406* at 25% load for various injection timings. The computational data have been obtained with and without the dissipation correction.

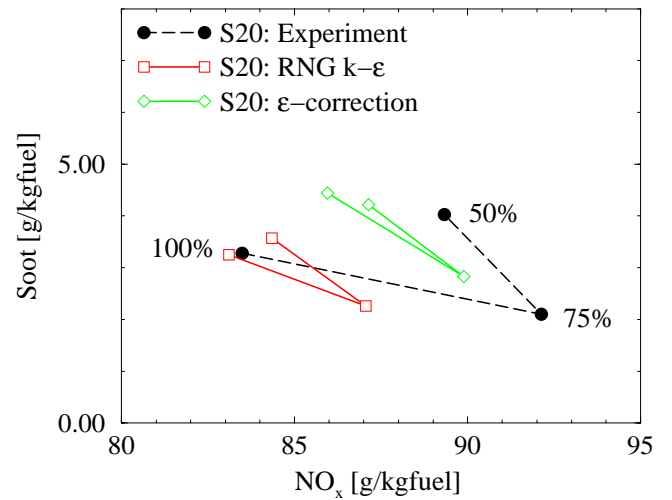


Figure 8. Soot- NO_x trade-off of the *Sulzer S20* for 100%, 75% and 50% load. The computational data have been obtained with and without the dissipation correction.

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