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# CFD Modeling of reactive turbulent flows in supercritical water oxidation reactors: modification of Eddy Dissipation approach for turbulence-chemistry interactions

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## Abstract

The aim of this work is to evaluate a new model taking into account the interaction between turbulence and chemistry in supercritical water media, in order to describe the oxidation reaction occurring in SuperCritical Water Oxidation (SCWO) processes. The properties of water in its supercritical state is intermediate between that of gas and liquids. As a consequence, usual species transport approaches in liquid or gas phases fail to accurately model the oxidation reaction in SCWO reactors with calculated temperature overprediction. Hence, a truncated eddy dissipation model with truncated turbulence cascade was created and tested on tubular and double shell stirred reactors using ANSYS Fluent software. This model was fitted with measured temperature profiles and degradation yields data and showed good agreement.

**Keywords:** Supercritical water oxidation, CFD modeling, turbulent flows, reaction kinetics, Eddy Dissipation model

## 1. Introduction

SuperCritical Water Oxidation (SCWO) is a promising technology developed for liquid radio-contaminated organic effluents destruction. Due to the properties of supercritical water, intermediate between liquid and gas, SCWO process converts organic compounds into carbon dioxide and water in very short residence times and degradation yields higher than 99.9 %. SCWO also avoids the formation of NO<sub>x</sub> and SO<sub>x</sub>, thanks to the moderate operating temperature compared with conventional combustion by incineration. Such characteristics allow the implementation of SCWO technology as compact continuous reactors.

Previous works carried out by the CEA consisted in using the Eddy Dissipation Concept (EDC) approach using ANSYS Fluent software. This model showed good agreement with the experimental temperature profiles obtained on a tubular reactor (Moussière et al. 2007), but overestimates the head temperature of the reactor by 15 % when it is applied on a stirred double-shelled reactor (Moussiere et al. 2012). Then, the Eddy Dissipation Model (EDM), considering chemical reaction as instantaneous (Magnussen and Hjertager 1977), was tested, but it did not manage to fill the gap between predictions and measurements. Another approach, suitable for reactions in liquid phase, exists in the literature: the Eddy Dissipation Model – Multiple Time Scale Turbulent Mixer (EDM-MTS) was developed by Baldyga (Baldyga 1989) and showed similar discrepancies.

The aim of this study is to address the influence of turbulence on reaction rate in supercritical water medium with a homemade model. Because the thermodynamic properties of supercritical water are intermediate between that of gas and liquids, a truncated model is created and tested on tubular and double shell stirred reactors. This model has a configurable multiplicative parameter used to fit with experimental temperature profiles.

## 2. Materials and methods

### 2.1. Experimental apparatus

The stirred double-shelled reactor consists of an external vessel made of type Stainless Steel 316L which can withstand high pressure, and a titanium inner tube confining aggressive species. Water and air are mixed then pre-heated in the annular space by four electric heaters. Inlet temperatures are measured by 5 thermocouples, three of which are placed along the titanium tube whereas the two others are placed in the inlet and outlet zones, respectively.

### 2.2. Model description

A 2-dimensional-axis-symmetric pattern, has been built to represent the reactor geometry. The hypothesis of an incompressible fluid has been made, considering that the Mach number, defined by the ratio of the fluid velocity over the sound speed, is below 0.1. Furthermore, the system is isobaric at 300 bar, pressure at which are calculated standard enthalpies of each species. Thermodynamic properties of every compound are calculated using a polynomial interpolation from NIST database and ideal mixing law is assumed. The rotation of the stirrer is simulated using Sliding Mesh Method by imposing a swirl velocity to the fluid instead of using a moving mesh, which is constructed with 230,000 cells. The turbulence model used is RNG k- $\epsilon$ .

The reaction (see Eq. (1)) kinetics are taken into account by a truncation of the EDM-MTS model. In this model, the concentration variance  $\sigma_s^2$  is divided into three parts, namely: the inertial-convective variance  $\sigma_1^2$ , the viscous-convective variance  $\sigma_2^2$  and the viscous-diffusive  $\sigma_3^2$  variance as in Eq. (2). This is an instant reaction model, in which reaction kinetics are governed by the transport of matter as in Eq. (3) (Hjertager et al. 2002).  $A_T$  is a multiplicative constant which can be configured to fit with experimental data. The truncation of the model only takes into account the viscous-convective variance.

### 3. Results

First, the EDM, EDM-MTS and truncated EDM-MTS models were compared, while keeping the model parameters constant. The results shown in Figure 1 indicates a slight improvement in wall temperature profile calculation with the EDM-MTS model: the location of the temperature peak is more accurately predicted but the deviation regarding its maximum temperature is still large, with a 14 % deviation versus 16 % obtained with the EDM. The truncated EDM-MTS model gives exactly the same results than the EDM with  $A_T = 1$ , but shows good agreement with experimental data, when the value of  $A_T$  is set on 0.005 or 0.01, as shown in Figure 2: the peak temperature deviation is nearly null for  $A_T = 0.005$ , and 2 % for  $A_T = 0.01$ . In this work, a more precise analysis is carried out to determine the optimal value of the multiplicative constant.

### 4. Equations, Figures and Tables

#### 4.1. Equations



$$\sigma_s^2 = \sigma_1^2 + \sigma_2^2 + \sigma_3^2 \quad (2)$$

$$R_A = -\frac{A_T \rho G_T \sigma_3^2}{2\sigma_s^2} \min\left(Y_A, \frac{Y_B}{s}\right) \quad (3)$$

#### 4.2. Figures

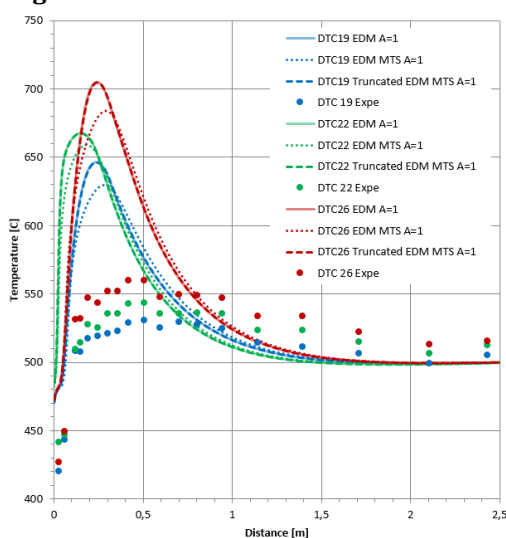


Figure 1 : Flowsheet of SCWO process (Moussiere et al. 2012)

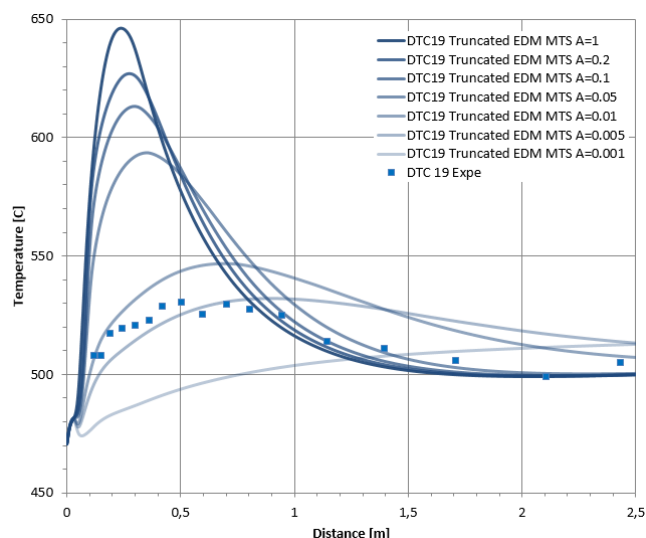


Figure 2 : Calculated temperature profiles (plain lines) along the reactor wall with different values for  $A_T$ , compared with experimental data (square dots)

### 5. Conclusions and perspectives

This study shows that the truncated EDM-MTS model is more suitable than the EDM and EDM-MTS models to take into account reaction kinetics, and that it is able to describe the interaction between turbulence and chemistry. Nonetheless, further research is needed to optimize the precision of this model. Moreover, it might be worthwhile to test the truncated EDM-MTS model on a three-dimensional geometry. Another modelling approach should be considered, using Probability Density Functions with Direct Quadrature Method of Moments - Interaction by Exchange with the Mean (DQMOM-IEM) model. However, the use of such an approach needs a better knowledge of kinetics laws in supercritical water conditions.

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