

# TOWARDS GENERIC REACTIVE FLOW MODELLING

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## INTRODUCTION

Simulation of reacting flows relies heavily on sub-models for chemistry and turbulence-chemistry interaction. The main problem employing these models is their, usually, limited range of validity [1-4]. Therefore, sub-models have to be thoroughly chosen and tested prior to employing them. However, complex reactive flows featuring different flow and chemistry regimes would need generic models capable of adapting to the occurring regimes. Such generic models might also improve the predictions for classical combustion problems. According to literature, generic models could be based on local flow and chemistry time scales [4]. Determining flow time scales is straight forward, while determining chemistry time scales is problematic [5-6]. Therefore, as a first step towards a more generic reactive flow modelling, a critical evaluation of the chemical time scales is done. Well known definitions of the chemical time scale ( $\tau_c$ ) were proposed e.g. by Rehm et al. [5] and Prüfert et al. [6]. Rehm et al. proposed two definitions, Rehm I (Eq. 1) is defined as the maximum of the inverse reaction rate Jacobian (J). Rehm II (Eq. 2), defines the chemical time scale as the maximum of the inverse of the real parts of the reaction rate Jacobian eigenvalues ( $\lambda_i$ ). Prüfert et al. [6] (Eq. 3) defined the chemical time scale as the inverse Euclidean matrix norm of the weighted reaction rate Jacobian. The weighting is done by the reaction rate ( $\omega_i$ ).

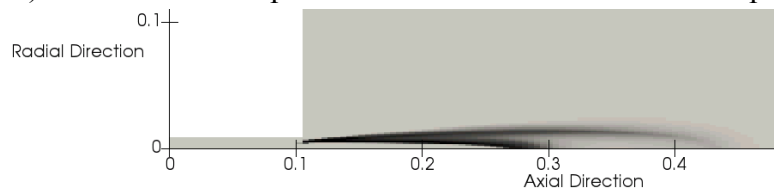
$$\tau_c = \max\left(\frac{1}{J}\right) \quad (1)$$

$$\tau_c = \max\left(\frac{1}{|\operatorname{Re}(\lambda_i)|}\right) \quad (2)$$

$$\tau_c = \left\| J_{ij} \frac{\omega_i}{\|\omega_{ij}\|} \right\|^{-1} \quad (3)$$

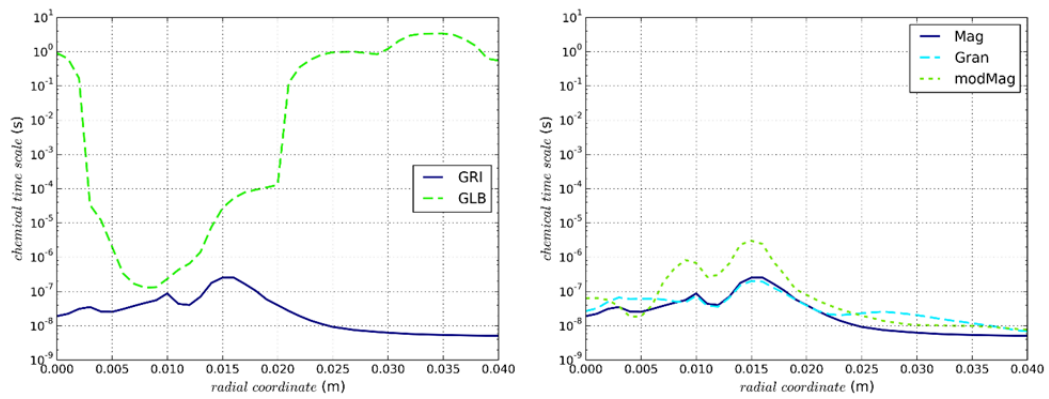
## TIME SCALE EVALUATION

The influences of the turbulence-chemistry interaction model, the reaction mechanism and the time scale definition on the chemical time scale are investigated. Therefore, the Eddy Dissipation Concept [1] (EDC) interaction model and two modifications (Gran [2] & modMag [3]), the comprehensive GRI [10] mechanism and a global reaction as well as the time scale definitions of Rehm et al. [5] and Prüfert et al. [6] were employed to model the well-known Sandia Flame D [7]. All 18 test cases were modelled with customized solvers based on the open source library OpenFOAM®. The chemical time scales were evaluated 0.1 m upstream of the burner tip. Figure 1 indicates the evaluation point (0.2 m axial direction) of the evaluation point and shows the methane consumption rate.

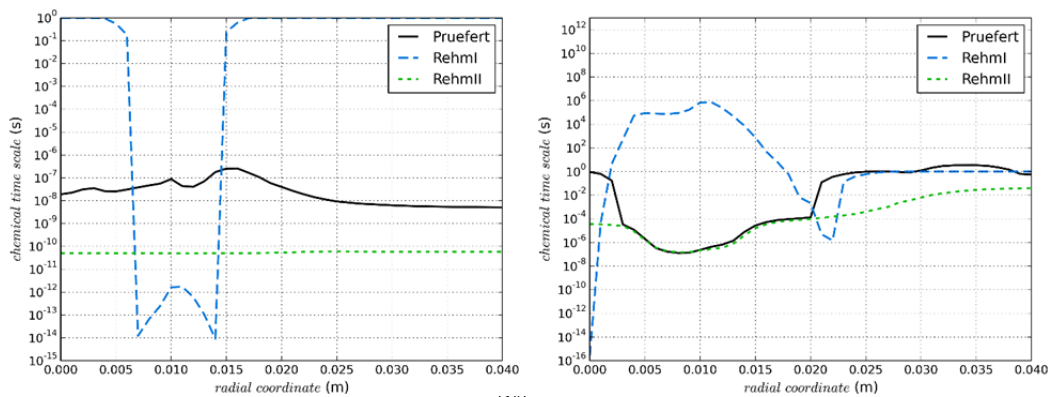


**Figure 1:** Reaction layer of the Flame D indicated by the methane consumption rate for the global reaction (black: high, grey: low; axial and radial direction in meters)

Figure 2 and Figure 3 compare the time scale dependencies on the reaction mechanism and the chemistry-turbulence model, and the time scale definitions, respectively. Reaction mechanism and time scale definition show a significant influence on the calculated time scales, while the chemistry-turbulence model has a minor influence.



**Figure 2:** Chemical time scale for different chemical reaction mechanism (left) and turbulence-chemistry interaction models (right) 0.1 m upstream the Sandia Flame D [8,9] burner tip; Time scale according to Prüfert et al. [7]



**Figure 3:** Chemical time scales for the GRI mechanism [10] (left) and a global one-step reaction (right) 0.1 m upstream the Sandia Flame D [8,9] burner tip; Time scale definitions by Rehm et al. [6] and Prüfert et al. [7]

## CONCLUSION

The assessment of the chemical time scale dependencies revealed a high influence of the reaction mechanism and the time scale definition. Differences are in the range of several orders of magnitude and the predicted time scale profiles along the radial coordinate feature different characteristics. Since generic modelling of reactive flows requires a reliable and consistent time scale prediction, further research effort has to be put on the definition of robust and reliable chemical time scale definitions. If these are available, reactive flow modelling might get improved by more generic models, especially, for complex multi-scale applications.

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