A novel methodology for Chemical Reactor Network extraction from CFD data via unsupervised clustering

Matteo Savarese[1,2], Alberto Cuoci[3], Ward De Paepe[2], Alessandro Parente[1]

1 Universite Libre de Bruxelles, Aero-Thermo-Mechanic department, Belgium
2 Université de Mons, Service de Termique et Combustion, Belgium
3 Politecnico di Milano, department of Chemistry, Materials and Chemical Engineering, Italy

Chemical Reactor Networks (CRN) are a modeling tool widely employed to predict pollutants emissions from realistic combustion systems. Their concept stem from the idea of dividing a combustion chamber into different zones and solving conservation equations for species and energy only in those few compartments, treated as canonical chemical reactors (i.e. perfectly stirred reactor or plug flow reactors), thus allowing for a drastic reduction of computational cost with respect to CFD, and detailed kinetics can be employed to account for pollutants formation. Since this tool rely on a schematic representation of a more complex flow field, the performances of those model are strongly affected by the adopted reactor configuration. Extracting the key features of the system flow field, and incorporating them in an equivalent CRN, is a trivial task, and most of literature examples rely on manual and trial-and-error procedures. in this work we present an automatic procedure for the extraction of equivalent CRN from CFD data, based on machine learning clustering algorithms. In this way, CFD data are post-processed in an unsupervised manner and the relevant zones in the combustor are identified. The volumes of the compartments and the mass flowrates across them are computed, and the resulting CRN is solved through an *ad-hoc* software using detailed kinetic mechanisms. The methodology is applied on a test case, a quasi-industrial, flameless-capable furnace fed with methane-hydrogen mixtures at different proportions. CRN predictions of emissions are then validated against experimental data.