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Computational modeling of combustion processes of diesel fuel serves as a practical tool to gain insight and to optimize the design of engines of tomorrow. However, in order to provide reliable predictions, models need to account for the detailed evolution of a large number of chemical species in addition to complex sub-processes such as turbulence and heat transfer occurring in an engine. This not only implies that the modeling of actual fuels is formidable, but also that much data is unavailable. Therefore resort could be made to surrogate fuels. These are simpler single or multi-component mixtures of defined composition with similar physical and chemical properties and combustion characteristics.

Models for n-dodecane, n-heptane, toluene and mixtures thereof have been studied with particular emphasis on ignition characteristics. Experiments have been carried out for a range of conditions such as on a four-cylinder diesel engine, in a combustion chamber with optical access connected externally to one cylinder with a modified piston. The experimental auto-ignition has been determined by means of pressure-time information and optical luminosity, using high speed imaging. The simulations have been carried out employing the SRM with DI module available in DARS with matching injection profiles as for the experiments. Kinetic models from literature have been reduced and implemented for the purpose of the CPU-intensive stochastic reactor modeling.

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