### Accepted Manuscript

#### **Research Paper**

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PII:	S1359-4311(16)33124-6
DOI:	http://dx.doi.org/10.1016/j.applthermaleng.2017.04.090
Reference:	ATE 10239
To appear in:	Applied Thermal Engineering
Received Date:	7 November 2016
Revised Date:	4 April 2017
Accepted Date:	20 April 2017



Please cite this article as: E. Neshat, D. Honnery, R.K. Saray, Multi-zone model for diesel engine simulation based on chemical kinetics mechanism, *Applied Thermal Engineering* (2017), doi: http://dx.doi.org/10.1016/j.applthermaleng.2017.04.090

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## ACCEPTED MANUSCRIPT

#### Multi-zone model for diesel engine simulation based on chemical kinetics mechanism

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#### Abstract

The main purpose of this study was to develop a new multi-zone model for simulating the diesel engine's closed loop. The proposed multi-zone model is based on chemical kinetics and uses a semi-detailed chemical kinetics mechanism containing 76 species and 327 reactions to calculate the fuel burning rate at each time step. This chemical kinetics mechanism contains 6 reactions to simulate soot formation and 14 reactions to simulate NOx formation. Prior to fuel injection, the combustion chamber is divided into three zones: inner zone, boundary layer zone, and crevice zone. The model considers the heat and mass transfers between the zones. Convective and radiation heat transfers are considered between the boundary layer zone and combustion chamber walls. When fuel injection begins, the spray is modeled and a zone is formed that contains the fuel jet. The geometry of the fuel jet zone is estimated using the spray-cone angle, and the length of this zone (fuel jet) is estimated using the Higgin's correlation. The spray-cone angle is calculated using the Reitz and Bracco's correlation. Fuel spray penetration into other zones is calculated using the Wakuri's relation. Fick's law is used to calculate the diffusion rate of different species in each zone. The model results are in good agreement with experimental data in predicting the

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