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Programa de Pós-Graduação em Engenharia Mecânica

METHODOLOGY FOR ANALYSIS OF BOUNDARY CONDITIONS IN ORDER TO INCREASE ACCURACY ASSOCIATED TO INTERNAL COMBUSTION ENGINE CFD 3D MODELS

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Tese submetida à Banca Examinadora designada pelo Colegiado do Programa de Pós-Graduação em Engenharia Mecânica da Universidade Federal de Minas Gerais, como parte dos requisitos necessários à obtenção do título de **"Doutor em Engenharia Mecânica"**, na área de concentração de **"Energia e Sustentabilidade".**

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Aos meus pais, Lincoln e Vânia;

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"...*rise and rise again, until lambs become lions*..." (Autor desconhecido. Robin Hood, 2010.)

ABSTRACT

The use of internal combustion engine simulation models for aiding the development of more efficient and less pollutant engines is by so far known. Engine CFD 3D models are a new tool for this development, although its methodology still needs some improvement in order to systematically produce accurate results. In this thesis, a method for analysis and treatment of boundary conditions for engine CFD 3D models using RANS approach is presented, which should be capable of producing accurate results for different engine operating conditions using the same values for all of the constants of the sub models for turbulence, spray and combustion, so the engine CFD 3D model would be used in a systematic and repetitive way. For intake pressure boundary conditions, a correction for pulsating flow effects is applied, and for wall temperature, the engine CFD 3D results for heat transfer coefficient are used decoupled iteratively with a zero dimensional heat transfer model. The method is applied to a naturally aspired single cylinder research engine available at CTM-UFMG, fueled with commercial ethanol, for which geometry information and experimental data are available. For the engine CFD 3D model with experimental data intake pressure boundary conditions, the results obtained for injected mass of fuel, lambda and trapped mass of air are compared to experimental data, and excess of air is observed for six different engine operating conditions. The results obtained by the engine CFD 3D model, using corrected intake pressure boundary conditions, are presented for injected mass of fuel, lambda and trapped mass of air for six different engine operating conditions, using two different sets of wall temperature boundary conditions calculated by the zero dimensional heat transfer model. For all of those results, the difference to experimental correlated data is systematically reduced in comparison with the direct use of experimental data for intake pressure boundary conditions. In cylinder pressure trace is compared between experimental data and three different sets of boundary conditions for two selected engine operating conditions, once the trends observed for the selected conditions are representative. The results obtained by the proposed method present better agreement to experimental correlated data than the direct use of experimental data for intake pressure boundary condition, specially during compression and expansion strokes. It is concluded that for this specific naturally aspired engine, pressure correction of intake experimental boundary conditions is mandatory for performing engine CFD 3D modelling using RANS approach. Once the method has been applied in only one engine, it is only possible to infer, and not to state, that pressure correction of intake experimental boundary conditions is mandatory for this application.

Keywords: CFD 3D, RANS, Internal Combustion Engines, Intake Pressure, Wall Temperature

RESUMO

O uso de modelos para simulação de motores de combustão interna, com objetivo de desenvolver motores mais eficientes e menos poluentes, é prática comum tanto na indústria quanto nos centros de pesquisa. Modelos CFD 3D para motores de combustão interna são uma nova ferramenta para esta aplicação, contudo sua metodologia ainda precisa de algum desenvolvimento para produzir sistematicamente resultados confiáveis. Nesta tese, é apresentada uma metodologia para análise das condições de contorno implementadas em modelos CFD 3D de motores de combustão interna que utilizam o tratamento RANS para turbulência, sendo que esta metodologia deve ser capaz de produzir resultados confiáveis para diferentes condições de operação do motor utilizando sempre os mesmos valores para todas as constantes dos sub modelos relacionados a turbulência, "spray" e combustão. Para condições de contorno de pressão na admissão, uma correção é aplicada aos dados experimentais devido ao efeito do escoamento pulsante na admissão, enquanto para as temperaturas de parede, os resultados do modelo CFD 3D para coeficiente de transferência de calor são usados de forma iterativa desacoplada com um modelo de transferência de calor zero dimensional. A metodologia é aplicada a um motor monocilindro de pesquisa aspirado disponível no CTM-UFMG, utilizando etanol comercial, em relação ao qual informações sobre geometria e dados experimentais foram disponibilizados para esta pesquisa. Para o modelo CFD 3D utilizando dados experimentais como condição de contorno de pressão na admissão, os resultados obtidos para massa de combustível injetada, lambda e massa de ar aprisionada são comparados com dados experimentais, e é constatado excesso de ar para seis diferentes condições de operação do motor. Os resultados obtidos pelo modelo CFD 3D, utilizando pressão corrigida como condição de contorno na admissão, são apresentados para massa de combustível injetada, lambda e massa de ar aprisionada para todos os casos, usando dois tipos de condição de contorno de temperatura de parede calculados pelo modelo zero dimensional de transferência de calor. Para todos os resultados, a diferença em relação aos dados experimentais correlatos é sempre menor que a obtida pelo uso direto dos dados experimentais de pressão na admissão como condição de contorno. Os resultados do modelo CFD 3D utilizando pressão corrigida como condição de contorno na admissão também apresentam melhor correlação com dados experimentais correlatos em comparação com os obtidos pelo mesmo modelo usando diretamente dados experimentais para a mesma condição de contorno, em termos do comportamento da pressão dentro do cilindro ao longo do ciclo e da temperatura dentro do cilindro ao longo do ciclo. Conclui-se que para o motor monocilindro aspirado em análise, a correção da condição de contorno de pressão na admissão é obrigatória para a modelagem CFD 3D de motores de combustão interna utilizando tratamento RANS para turbulência.

Palavras chave: CFD 3D, RANS, Motores de Combustão Interna, Pressão da Admissão, Temperatura de Parede

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NOMENCLATURE

Abbreviations

CO_2	Carbon Dioxide
NO_X	Generic Nitrogen Oxide
0D	Zero Dimensional
1D	One Dimensional
2D	Two Dimensional
3D	Three Dimensional
AKTIM	Ark and Kernel Tracking Ignition Model
ANSYS	Trade name of ANSYS INC.
ASME	The American Society of Mechanical Engineers.
BDC	Bottom Dead Center
CAD	Crank Angle Degrees
CCV	Cycle to Cycle Variations
CFD	Computational Fluid Dynamics
CFX	Trade name of a commercial software, which actually belongs to ANSYS INC.
CHT	Conjugate Heat Transfer
COV	Co Variance
CTM	*Centro de Tecnologia da Mobilidade*, (Mobility Technology Center, from Portuguese)
dim	Dimensionless
DISI	Direct Injection Spark Ignition
DNS	Direct Numerical Simulation
ECFM-3Z	Extended Coherent Flame Model - Three Zones
EGR	Exhaust Gas Recirculation

HPC	High Performance Computing
HT	Heat Transfer
ICE	Internal Combustion Engines
IMEP	Indicated Mean Effective Pressure
KIVA	Trade name of an open source software
KIVA-3V	Trade name of an open source software
LES	Large Eddy Simulation
PDF	Probability Density Function
PISO	Pressure Implicit with Splitting of Algorithm
PIV	Particle Image Velocimetry
RANS	Reynolds Averaged Navier Stokes
RNG	Re Normalization Group
SGS	Sub Grid Scale
STAR-CD	Trade name of a commercial software, which actually belongs to SIEMENS GmBH.
TDC	Top Dead Center
THC	Total Hydrocarbon
UFMG	*Universidade Federal de Minas Gerais* (Federal University of Minas Gerais, from Portuguese)

Greek symbols

α	ECFM-3Z model constant [-]
β	ECFM-3Z model constant [-]
$\delta(Z)$	Probability density function for unmixed air zone [-]
$\delta(Z-1)$	Probability density function for unmixed fuel zone [-]
$\delta(Z-\overline{Z}^M)$	Probability density function for mixture zone [-]
ε	Dissipation of turbulent kinetic energy $[m^2/s^3]$

ε_{cyl}	Weighting factor for heat transfer between valve stem surface and port gas flow, for which the reference is the heat transfer modeled as flow past a cylinder
$\overline{\rho}$	Flow field average density $[kg/m^3]$
ϕ	Generic trasport variable [-]
ϕ_{i+1}	Value of the generic variable ϕ at grid $i+1$ [-]
ϕ_i	Value of the generic variable ϕ at grid i [-]
Σ	Flame surface density $[m^2/m^3]$

Latin symbols

$\overline{I}$	Flow field average total internal energy $[kJ]$
$\overline{P}$	Flow field average pressure $[Pa]$
$\overline{T}$	Flow field average temperature $[K]$
$\overline{U}$	Flow field average velocity component $[m/s]$
$\overline{V}$	Flow field average velocity component $[m/s]$
$\overline{W}$	Flow field average velocity component $[m/s]$
$\overline{Z}^M$	Average Mixture Fraction [-]
$\vec{\overline{U}}$	Flow field average velocity vector $[m/s]$
A	Air plus Exhaust Gas Recirculation Zone [-]
A_{cc}	Area of the combustion chamber for the global heat transfer model $[m^2]$
A_{exh}	Area of the exhaust port for the global heat transfer model $[m^2]$
A_{int}	Area of the intake port for the global heat transfer model $[m^2]$
$A_{lin,ext}$	Area of cylinder outside surface exposed to coolant flow $[m^2]$
c	Reaction progress variable [-]
C'_{gal}	Constant in the equation for thermal conductance between piston surface and oil [-]
C_2	Constant in the Woschni equation [-]
C_u	Constant in the Woschni equation [-]

C_{w1}	Constant in the Woschni equation [-]
C_{w2}	Constant in the Woschni equation [-]
D	Generic experimental measurement [-]
D_{curv}	Port curvature diameter $[m]$
D_{cyl}	Cylinder diameter (bore) in the Woschni equation $[m]$
D_{gal}	Piston inner diameter in the region of the lubricating oil gallery $[m]$
d_{gal}	Diameter or hydraulic diameter of the piston lubricating oil gallery $[m]$
D_{pis}	Piston diameter $[m]$
D_{port}	Port diameter or hydraulic diameter $[m]$
E	Generic comparison error [-]
e_{cc}	Thickness of the combustion chamber for the global heat transfer model
e_{exh}	Thickness of the exhaust port for the global heat transfer model
e_{int}	Thickness of the intake port for the global heat transfer model
e_{lin}	Thickness of the cylinder wall for the global heat transfer model
F	Unburned Fuel Zone [-]
h	Grid characteristic length $[mm]$
h_{coarse}	Characteristic length of a coarse grid $[mm]$
$h_{cylinder}$	Heat transfer coefficient between valve stem surface and port gas flow, modeled as flow past a cylinder $[W/m^2K]$
h_{fine}	Characteristic length of a fine grid $[mm]$
$h_{flatplate}$	Heat transfer coefficient between valve stem surface and port gas flow, modeled as flow past a flat plate $[W/m^2K]$
$h_{gal-cool}$	Heat transfer coefficient between head cooling gallery surface and coolant flow $[W/m^2K]$
h_{gas}	Heat transfer coefficient for in cylinder gas $[W/m^2K]$
$h_{lin-cool}$	Heat transfer coefficient between cylinder outside surface and coolant flow $[W/m^2K]$

$h_{lin-oil}$	Heat transfer coefficient between cylinder liner surface and oil $[W/m^2K]$
h_{pc}	Piston ring height $[m]$
$h_{pis-lin}$	Heat transfer coefficient between piston surface and cylinder liner surface $[W/m^2K]$
$h_{portcurv}$	Heat transfer coefficient between port surface and port gas flow, for curved tube approximation $[W/m^2K]$
$h_{stemgas}$	Heat transfer coefficient between valve stem surface and port gas flow $[W/m^2K]$
$h_{straighttube}(x=\infty)$	Heat transfer coefficient between port surface and port gas flow, for straight tube approximation in fully developed flow $[W/m^2K]$
k	Turbulent kinetic energy $[m^2/s^2]$
K_{cc-gal}	Thermal conductance between combustion chamber surface and head cooling gallery surface $[W/K]$
k_{cc}	Thermal conductivity of the cylinder wall, for the global heat transfer model $[W/m.K]$
k_{cc}	Thermal conductivity of the engine head in the region of the combustion chamber, for the global heat transfer model $[W/m.K]$
$K_{exh-gal}$	Thermal conductance between exhaust port surface and head cooling gallery surface $[W/K]$
k_{exh}	Thermal conductivity of the engine head in the region of the exhaust port, for the global heat transfer model $[W/m.K]$
$K_{gal-cool}$	Thermal conductance between head cooling gallery surface and coolant flow $[W/K]$
$K_{gas-head}$	Thermal conductance between in cylinder gases and combustion chamber surface $[W/K]$
$K_{gas-lin}$	Thermal conductance between in cylinder gases and cylinder liner surface $[W/K]$
$K_{gas-pis}$	Thermal conductance between in cylinder gases and piston surface $[W/K]$
$K_{gas-valv}$	Thermal conductance between in cylinder gases and valve surface $[W/K]$
$K_{int-gal}$	Thermal conductance between intake port surface and head cooling gallery surface $[W/K]$

k_{int}	Thermal conductivity of the engine head in the region of the intake port, for the global heat transfer model $[W/m.K]$
$K_{lin-cool}$	Thermal conductance between cylinder liner surface and coolant flow $[W/K]$
$K_{lin-oil}$	Thermal conductance between cylinder liner surface and oil $[W/K]$
$K_{pis-lin}$	Thermal conductance between piston surface and cylinder liner surface $[W/K]$
$K_{pis-oil}$	Thermal conductance between piston surface and oil $[W/K]$
k_{pis}	Thermal conductivity of the piston, for the global heat transfer model $[W/m.K]$
M	Mixture Zone [-]
m	Constant in the equation for thermal conductance between piston surface and oil [-]
N	Total number of finite volumes in a grid [-]
$Nu_{cylinder}$	Nusselt number for heat transfer between valve stem and port gas flow, modeled as flow past a cylinder [dim]
$Nu_D(x)$	Nusselt number for heat transfer between port surface and port gas flow, for turbulent entrance length flow [dim]
$Nu_D(x=\infty)$	Nusselt number for heat transfer between port surface and port gas flow, for turbulent fully developed flow [dim]
$Nu_{flatplate}$	Nusselt number for heat transfer between valve stem and port gas flow, modeled as flow past a flat plate [dim]
p_{ivc}	Pressure of the in cylinder gases at intake valve closing [bar]
r	Grid refinement ratio [dim]
Re	Reynolds number [dim]
S	Generic simulation result [-]
S_{cyl}	Cylinder stroke $[m]$
S_p	Average piston speed for the global heat transfer model [-]
$T_{gas-head}$	Cycle average in cylinder gas temperature, as it is seen by combustion chamber surface [K]

$T_{gas-lin}$	Cycle average in cylinder gas temperature, as it is seen by cylinder liner surface [K]
$T_{gas-pis}$	Cycle average in cylinder gas temperature, as it is seen by piston surface [K]
$T_{gas-valv}$	Cycle average in cylinder gas temperature, as it is seen by valve surface [K]
T_{ivc}	Temperature of the in cylinder gases at intake valve closing [K]
$U_{95\%}$	Uncertainty of a given result, for a 95% confidence interval [-]
V_D	Displaced volume in the Woschni equation [-]
V_{ivc}	Volume of the in cylinder gases at intake valve closing [m^3]
V_i	Volume of the i_{th} cell [mm^3]
x	Port length for heat transfer between port surface and port gas flow [m]
Z	Mixture fraction variable [-]
P _1aIT	Results for in cylinder pressure trace obtained by engine CFD 3D model using fitted intake pressure boundary conditions along with first iteration wall temperatures calculated by global heat transfer model [bar]
P _2aIT	Results for in cylinder pressure trace obtained by engine CFD 3D model using fitted intake pressure boundary conditions along with second iteration wall temperatures calculated by global heat transfer model [bar]
P _envelope	Experimental data for in cylinder pressure, associated to the dispersion of the 200 cycles for in cylinder pressure experimental data [bar]
P _EXP	Experimental data for in cylinder pressure trace [bar]
P _max	Maximum pressure of in cylinder pressure trace (peak pressure) [bar]
P _piexp	Results for in cylinder pressure trace obtained by engine CFD 3D model using experimental data intake pressure boundary conditions along with first iteration wall temperatures calculated by global heat transfer model [bar]

CONTENTS

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