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Micro-article

Turbulent uniformity fluctuations in automotive catalysts – A RANS vs DES assessment

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ABSTRACT

Attaining sufficient flow uniformity in catalytic aftertreatment systems is a major challenge for the automotive industry. Computational fluid dynamics (CFD) simulations offer means of analyzing and quantifying this flow uniformity *in silico*. In this work, predictions from numerical simulations of flow uniformity obtained using a conventional steady-state Reynolds-Averaged Navier-Stokes (RANS) approach are contrasted against comprehensive Detached Eddy Simulations (DES) where the large-scale turbulence is resolved in space and time. It is shown that the DES approach provides access to data on flow uniformity fluctuations that could be significant for the catalyst light-off behavior. However, the computational cost of the DES is approximately three orders of magnitude larger than that of the corresponding RANS simulation.

1. Introduction

Computational fluid dynamics (CFD) simulations of automotive components, such as exhaust gas systems, have the potential to provide detailed insight into their performance [1–6]. This performance is usually expressed in terms of conversion and uniformity index [7], which are scalar quantities that may be directly obtained from CFD data. The conventional approach is to use a Reynolds-Averaged Navier-Stokes (RANS)-based model to determine the uniformity indices from the mean velocity and temperature fields [7–13]. With a more sophisticated scale-resolving turbulence model, it would be possible to also resolve the turbulent uniformity index fluctuations (cf [14,15]). The aim of the current work is to employ a Detached Eddy Simulation (DES) strategy and contrast it to a baseline RANS approach for resolving the effect of turbulent fluctuations on the flow uniformity index in a geometrically complex automotive exhaust gas aftertreatment system.

2. Methodology

To obtain the velocity and temperature fields at the exit of the catalytic converter, one RANS and one DES case are performed using ANSYS Fluent 2022 R1 [16]. The geometry is detailed in our previous work [17] (cf. Fig. 1A), and the differences in the two case setups are specified in Table 1. The fluid properties are taken to be those of air. The inlet velocity is 25 m/s, the inlet temperature is 423 K, the inlet turbulence intensity is 4%, and the inlet turbulent length scale is 0.01 m. A pressure-outlet boundary condition is applied on the outlet with 0 Pa gauge pressure. Heat losses prescribed to match with experiments [17] are used at the bounding walls. The flow is non-reactive. The DES is initiated from the RANS solution by superimposing sampled fluctuations. The velocity field is used to determine the flow uniformity index [16].

3. Results and discussion

The RANS simulation predicts a steady uniformity index of 0.92, whereas the time-averaged prediction from the DES is 0.93 after $>$ 1 s of sampling. The flow uniformity index in the DES (cf. Fig. 1C) exhibits oscillations between 0.87 and 0.95 on time scales similar to the retention time through the flow domain (0.125 s).

The turbulent fluctuations in flow uniformity obtained from the DES is $\pm$4.3%, which is comparable to the turbulence intensity (4%). This level of uniformity fluctuations should be sufficient to produce skewed conversion fluctuations, owing to the non-linear dependence of chemical conversion on the local residence time in the catalyst brick [7]. Such effects are most pronounced for reactions with negative-order kinetics

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when operating close to ignition or extinction [18], implying that the influence of turbulent uniformity fluctuations would be most pronounced during critical events such as catalyst light-off for CO oxidation.

It is evident that there is a slight asymmetry in the DES results (cf. Fig. 1D), which indicates that the > 8 flow-through times simulated are somewhat insufficient for full convergence of the statistics. Even so, both simulations produce qualitatively similar pictures, with a crescent high-speed region at the bottom of the catalyst brick and a more rounded low-speed region, flanked by higher-velocity streaks, discernible in the upper part. When DES snapshots of the velocity field at low uniformity are contrasted to snapshots at high uniformity (cf. Fig. 1E), similar patterns emerge and re-emerge as the turbulence generation from the flow discharging from the smaller vertical pipe before the catalyst (cf. Fig. 1A) causes an inherent unsteadiness of the flow.

Finally, the computational cost for the two turbulence treatments is also assessed. The DES is considerably more costly than the RANS due to the larger mesh and the need for a transient solution. More specifically, whereas the RANS results could be obtained in 26 core hours, the DES required more than 20,000 core hours – an increase of almost three orders of magnitude.

Table 1
CFD case specifications.

Setting	RANS	DES
Turbulence model	SST k-ω	SST k-ω-based [16]
Mesh size	1.2 million cells	6 million cells
Time stepping	None (steady state)	$\Delta t = 0.0001$ s

4. Conclusions

The flow uniformity in a catalyst brick in an automotive aftertreatment system was predicted using CFD simulations, in which steady-state RANS was contrasted with DES (both based on the SST k-ω model). The obtained mean fields were in good agreement. Unlike the RANS approach, the DES methodology enables the resolution of turbulent fluctuations in uniformity with time. These fluctuations contain a mixture of high- and low-frequency contributions, and could be expected to influence the chemical conversion, especially during critical

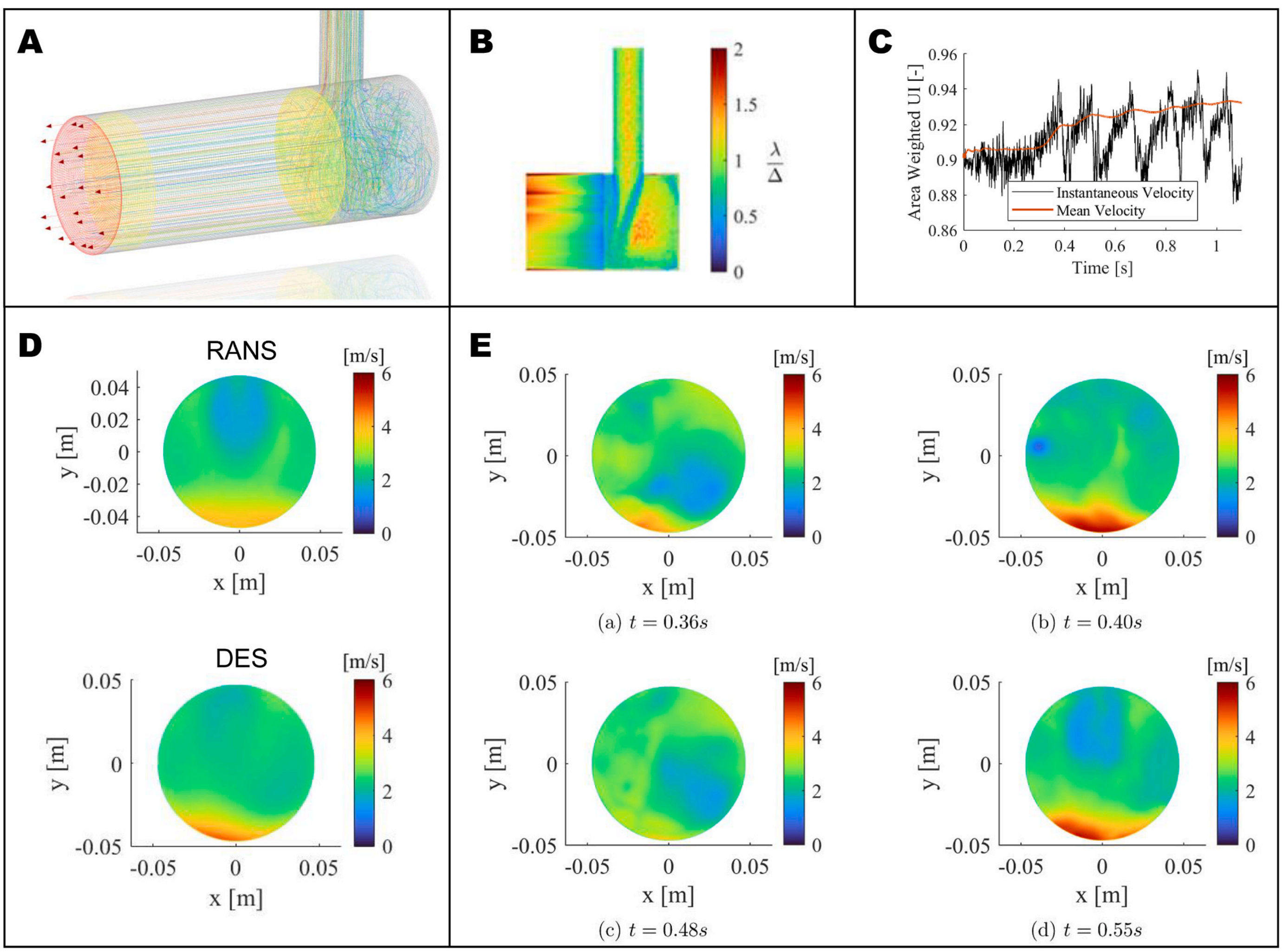

Fig. 1. Flow uniformity in a non-isothermal automotive aftertreatment system. A) Illustration of the geometry. The flow comes from above through a vertical inlet pipe and discharges into a horizontal pipe where the catalyst brick (yellow inlet and outlet planes) is positioned. The flow outlet is seen to the left. B) The mesh resolution in the DES upstream the catalyst entrance, expressed as the ratio of the Taylor length scale (λ) to the cell side length (Δ). C) The area-weighted flow uniformity index for the instantaneous velocity field (black line) and the mean velocity field (red line) in the DES as a function of time, at the catalyst mid-section. The simulation starts at t = −0.25 s, and sampling of statistics is initiated at t = 0 s. The mean velocity field is obtained by averaging over snapshots from t = 0 s onwards. D) Mean velocity magnitude contour plots for the RANS (top) and DES (bottom) simulations. E) Four snapshots from the DES (at t = 0.36 s and 0.48 s, corresponding to high uniformity, and t = 0.40 and 0.55 s, corresponding to low uniformity). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

events such as catalyst light-off. However, their resolution via DES is approximately three orders of magnitude more computationally costly than a conventional steady-state RANS simulation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

References

[1] I. Cornejo, P. Nikrityuk, R.E. Hayes, Pressure correction for automotive catalytic converters: a multi-zone permeability approach, Chem. Eng. Res. Des. 147 (2019) 232–243.

[2] I. Cornejo, P. Nikrityuk, R.E. Hayes, The influence of channel geometry on the pressure drop in automotive catalytic converters: model development and validation, Chem. Eng. Sci. 212 (2020), 115317.

[3] M. Prantoni, S. Aleksandrova, H. Medina, S. Benjamin, Multi-channel modelling approach for particulate filters, Res. Eng. 5 (2020), 100077.

[4] L. Teodosi, F. Timpone, G.N. dell'Annunziata, A. Genovese, RANS 3D CFD simulations to enhance the thermal prediction of tyre thermodynamic model: a hierarchical approach, Res. Eng. 12 (2021), 100288.

[5] F. Haq, J. Huang, Parametric design and IR signature study of exhaust plume from elliptical-shaped exhaust nozzles of a low flying UAV using CFD approach, Res. Eng. 13 (2022), 100320.

[6] C.R. Jadhav, R.P. Chorage, Modification in commercial bus model to overcome aerodynamic drag effect by using CFD analysis, Res. Eng. 6 (2022), 100091.

[7] P. Chanda Nagarajan, H. Ström, J. Sjöblom, Numerical assessment of flow pulsation effects on reactant conversion in automotive monolithic reactors, Catalysts 12 (2022) 613.

[8] H. Weltens, H. Bressler, F. Terres, H. Neumaier, D. Rammoser, Optimisation of catalytic converter gas flow distribution by CFD prediction, SAE Tech. Pap. (1993), 930780.

[9] A. Holmgren, T. Grönstedt, B. Andersson, Improved flow distribution in automotive monolithic converters, React. Kinet. Catal. Lett. 60 (1997) 363–371.

[10] G. Agrawal, N.S. Kaisare, S. Pushpavanam, K. Ramanthan, Modeling the effect of flow mal-distribution on the performance of a catalytic converter, Chem. Eng. Sci. 71 (2012) 310–320.

[11] S. Dammalapati, P. Aghalayam, N. Kaisare, Modeling the effects of the inlet manifold design on the performance of a diesel oxidation catalytic converter, Ind. Eng. Chem. Res. 60 (2021) 3860–3870.

[12] M. Mu, J. Sjöblom, H. Ström, X. Li, Analysis of the flow field from connection cones to monolith reactors, Energies 12 (2019) 455.

[13] V. Chakravarthy, J. Conklin, C. Daw, E. D'Avenzo, Multi-dimensional simulations of cold-start transients in a catalytic converter under steady inflow conditions, Appl. Catal. A: Gener. 241 (2003) 289–306.

[14] I. Cornejo, P. Nikrityuk, C. Lange, R.E. Hayes, Influence of upstream turbulence on the pressure drop inside a monolith, Chem. Eng. Process. – Process Intensif. 147 (2020), 107735.

[15] R. Vinuesa, High-fidelity simulations in complex geometries: towards better flow understanding and development of turbulence models, Res. Eng. 11 (2021), 100254.

[16] ANSYS, Inc, Ansys Fluent Theory Guide, Release, Canonsburg, U.S.A, 2022, 2022 R1.

[17] P. Chanda Nagarajan, H. Ström, J. Sjöblom, Transient flow uniformity evolution in realistic exhaust gas aftertreatment systems using 3D-CFD, Emiss. Contr. Sci. Technol. 8 (2022) 154–170, https://doi.org/10.1007/s40825-022-00217-6.

[18] H. Ström, S. Sasic, Heat and mass transfer in automotive catalysts – the influence of turbulent velocity fluctuations, Chem. Eng. Sci. 83 (2012) 128.