Using Computational Modeling to Design Cleaner, More Fuel-Efficient Motor Vehicles

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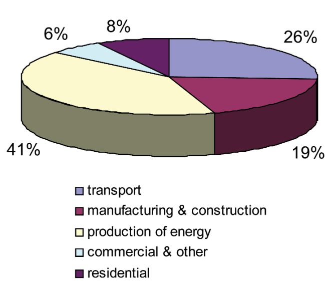
Introduction

Today's motor vehicles that use conventional fuel contribute substantially to air pollution and global warming, yet it is virtually impossible to imagine the modern world without these vehicles. In fact, the worldwide fleet will only increase in years to come, so we can expect that emission standards will continue to get progressively tighter in order to protect the environment and human health. We can also predict a related surge in the worldwide demand for oil to propel all of these vehicles. With two out of every three people now concerned about global warming, and governments concerned with the economic and political implications of rising oil prices, new powertrain technologies are needed to deliver zero, or near zero, emissions in addition to improved fuel economy. Replacement of conventionally powered vehicles with alternatively powered vehicles will likely accelerate as the new powertrain technologies mature. In the meantime, the focus will remain on improving the existing, conventional engine designs and relying on aftertreatment devices to clean up emissions. Computational fluid dynamics (CFD) software can play a valuable role in identifying cleaner, more fuel-efficient alternatives that improve engine designs. This paper discusses the scope and impact of the problem, and explains how CFD can be used to analyze emission-controlling devices and contribute to the achievement of emission standards.

Situation Overview

Motor vehicles represent one of the prime sources of air pollution in urban areas. They are responsible for more than 80% of carbon monoxide, for more than 55% of nitrogen oxides emissions, and for more than 40% of volatile organic compound emissions[1]. Motor vehicles are also a substantial contributor to greenhouse gas emissions, which affect the global climate. The International Energy Agency (IEA) estimates that the transportation sector is responsible for about 26% of global carbon emission (Chart 1), with the sector's emissions rising by 75% between 1997 and 2020. Reducing vehicle emissions will therefore play a crucial role in stabilizing atmospheric concentrations of greenhouse gases.

Chart 1:
Global Greenhouse Gas Emissions
Source: IEA[2]



The number of vehicles produced annually has been growing steadily over the past few decades from about 5 million worldwide just after World War II to about 55 million today[2]. It is expected that the trend of continued growth in the world's population and rapid industrialization of countries, especially in Asia, will lead to further increase in the worldwide fleet. The resulting vehicle emissions could seriously threaten air quality, global climate, and human health. For all the obvious benefits that motor vehicles provide to people, there are also severe drawbacks: ever-increasing fuel consumption, greater emission of air pollutants, and greater exposure to hazardous pollution, which causes serious health problems to people.

Health and Environmental Impacts

Air pollution kills 800,000 people each year, according to the World Health Organization[3]. In the United States, about 90 million people live in areas with air quality below the National Ambient Air Quality Standards[4]. Medical research has linked air pollution to a host of public health concerns including asthma, cancer, heart disease, high blood pressure, birth defects and brain damage, among others[5]. The American Lung Association estimated in 1988 that Americans paid more than $50 billion annually for health problems due to air pollution[1]. The cost is considerably higher today, due to rising healthcare fees and improved understanding of the impact of emissions on the human body.

In parallel, the atmospheric concentration of carbon dioxide (CO_2, aka "greenhouse gas") has increased by more than 30% since pre-industrial times, mostly due to the burning of fossil fuels. The resulting change in the global climate poses further risk to human health, through air- and water-borne illnesses, decreased production of staple foods, heat waves, cold spells, flooding, etc. The climate change may also have implications on national-security, as evident from the report prepared for the US Department of Defense[6].

Lancet Medical Journal Study

In Austria, France, and Switzerland:

- About 6% of all deaths, about 40,000 per year (twice the annual deaths from traffic accidents), are due to outdoor air pollution.
- Vehicles are responsible for about half of this total.
- People in cities die about 18 months earlier than they otherwise would.
- Each year, outdoor air pollution causes over 25,000 new cases of chronic bronchitis; 800,000 episodes of asthma and bronchitis; 16 million lost person days of activity per year.
- Health costs from traffic pollution are about 1.7% of total GDP.

Source: *The Lancet*, Vol. 356, Issue 9232, September 2000, pp 792, 795

Regulatory Landscape for Motor Vehicle Emissions

Motor vehicle emissions can be classified in two categories: *tailpipe emissions* and *evaporative emissions*. Tailpipe emissions are the by-product of engine combustion, while evaporative emissions result from fuel tank venting and refueling losses. The major tailpipe emission pollutants include hydrocarbons (volatile organic compounds, or VOCs, which contribute to smog), nitrogen oxides (NO_x contributes to smog and acid rain), carbon monoxide (poisonous gas) and carbon dioxide (greenhouse gas).

In the United States, emission standards are managed by the Environmental Protection Agency (EPA) or individual state governments. Currently, vehicles sold within the US, regardless of fuel type, must meet Tier II standards. Within the Tier II ranking, there are 10 emission levels called "Bins," with Bin-1 being the cleanest. Bin-5 represents the overall average that each automaker's fleet must meet. Starting January 1, 2007, the state of California, the largest US market, will impose even more stringent standards known as Low Emission Vehicle (LEV) II. LEV II will require every new vehicle sold in the state to be Bin-5 compliant.

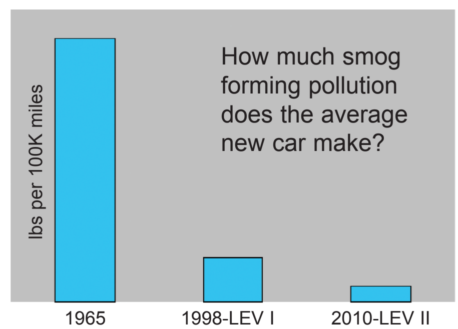


Chart 2: A new 1965 car produced about a ton of smog-forming hydrocarbons during 100,000 miles of driving. California's low-emission standards have cut that to around 50 pounds for the average 1998 car. LEV II would further reduce emissions from the average new 2010 car to approximately 10 pounds.[7]

Chart 3 (below): Average annual emissions - 2000 data, per EPA[8]

Passenger Car

COMPONENT	Total Annual Pollution Emitted and Fuel Consumed
Hydrocarbons	77.1 pounds of hydrocarbons
Carbon Monoxide	575 pounds of carbon monoxide
Oxides of Nitrogen	38.2 pounds of oxides of nitrogen
Carbon Dioxide	11,450 pounds of carbon dioxide
Gasoline	581 gallons of gasoline

Light Truck

COMPONENT	Total Annual Pollution Emitted and Fuel Consumed
Hydrocarbons	108 pounds of hydrocarbons
Carbon Monoxide	854 pounds of carbon monoxide
Oxides of Nitrogen	55.8 pounds of oxides of nitrogen
Carbon Dioxide	16,035 pounds of carbon dioxide
Gasoline	813 gallons of gasoline

Industry Landscape

In the US, the transportation sector is heavily dependent on petroleum fuel: 97% of the total fuel consumed by the sector is petroleum-based. Further, the sector consumes two-thirds of all US oil. Two of the main energy challenges facing the nation in the 21st century are reducing dependence on petroleum imports, and reducing pollution and greenhouse gas emissions[9].

While the long term goal is to develop vehicle technologies that do not require petroleum fuels, the interim focus is on reducing petroleum consumption by making vehicles more energy-efficient[1]. To this end, the auto manufacturers have been investing in the development of alternative technologies such as hybrid-electric, electric, fuel cell, and clean diesel powered vehicles. While these technologies are in various states of maturity, each retains some level of technical limitation that has yet to be ironed out. Electric and fuel cell powered vehicles are emission-free; however, their range at present is very limited, precluding them as a viable commercial technology. Hybrid-electric vehicles (HEVs) provide good fuel economy, but rely on expensive battery packs with a limited lifetime. The price of a new battery pack, currently about $3000, can be unsettling to prospective buyers. Diesel is the most mature technology, but in operation it produces a high level of tailpipe emissions.

Despite heavy investment by US auto makers, HEV technology is not expected to surpass the popularity of mainstream internal combustion engines over the next decade. The majority of US auto buyers believe that the path to cleaner air and better fuel economy lies in improving existing engine technology. Perhaps this explains why the US market share of diesel-powered vehicles is projected to nearly triple over the next 10 years from 3.2% in 2005 to more than 10% by 2015, while HEVs will have only 4.9% share of the market by 2013[10]. In other words, there could be two diesel vehicles for every HEV on US roads in the near future.

> **"We're very optimistic (about the future of diesels). This decade will be known for the transformation of the diesel engine, similar to how gasoline engines were revolutionized in the 1970s."[11]**
>
> Margo Oge, Director,Office of Transportation and Air Quality, US EPA

Diesels are popular in western Europe because of their fuel efficiency. They deliver about 30% better fuel economy than gasoline engines. Diesel's appeal in the US market lies in its ability to deliver high torque, a desirable powertrain feature for light-duty trucks (LDT) which represent a large segment of the market. In addition, diesel engine technology is mature, proven and perceived by customers as a "safe" purchase when considering warranty issues.

While diesels have a leg up on the gasoline engine in fuel efficiency and performance, they fail to burn as clean as gasoline engines. Diesels produce significantly more NO_x and particulate matter (PM) than gasoline engines due to the higher temperatures and pressures in their combustion cycle. The focus of "clean diesel technology" efforts is on reducing NO_x emissions by lowering the temperature of the diesel-combustion process. Large investments are required to develop a new diesel engine. The cost can be twice that of a conventional gasoline engine running upwards of $500 million to $1 billion[11], not to mention the significant time required to develop new engine technology. Until clean diesel technology becomes commercially available, existing diesel engines must be fit with cleaning equipment that controls emissions. Exhaust system aftertreatment technologies such as oxidation catalysts, particulate filters, and selective catalytic reduction (SCR) that are currently in use are intended to meet progressively tighter emission standards. Case in point: neither the American 2007 heavy truck engine emissions regulations, nor the European Union 2007 automobile regulations, can be met without aftertreatment devices.

How Simulation Helps the Cause

Regardless of what type of underlying powertrain system is used, buyers ultimately expect vehicles that deliver on fuel economy and meet emission targets without sacrificing performance, comfort, and price. Such market requirements put substantial pressure on auto manufacturers to be able to accelerate the development and testing cycles of multiple alternatives in a cost-efficient way. Computer-aided engineering (CAE) software has been widely embraced by the auto industry for its ability to help bring new or improved products to the market faster and at less cost. As a virtual simulation tool, CAE helps to “prune” the myriad of possible design alternatives and to identify the most promising performers. Computational fluid dynamics (CFD) is a valuable tool in the CAE solution toolkit. It enables the modeling of fluid flow related phenomena. CFD can help with understanding fluid, thermal, and chemical processes occurring inside or outside a vehicle including the processes associated with conventional (gasoline or diesel) and alternative (hybrid-electric and fuel cell) powertrain systems. For example, conventional engines are analyzed with CFD to obtain performance data such as specific fuel consumption and emission indexes. Likewise, HEV thermal management of components such as battery packs, motors, and power electronics can be evaluated using CFD, along with applications such as species dispersion due to battery leakages. Following are examples of how fluid flow modeling is being used successfully to improve effectiveness of emission-controlling devices in conventional powertrain systems.

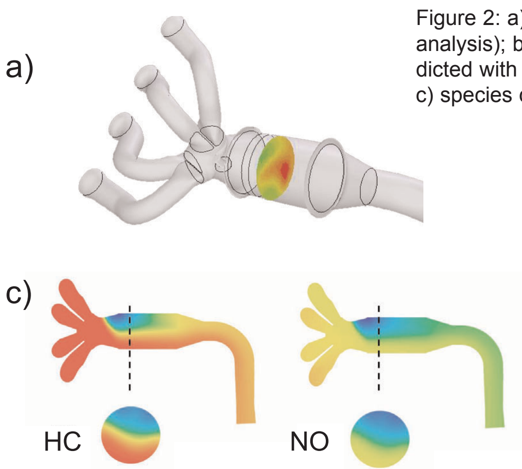
Figure 1: Transient investigation of swirling in-cylinder flow in a diesel engine
Courtesy of Deutz AG

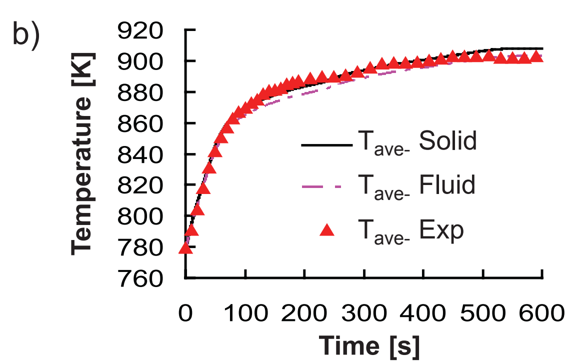
Example 1: Catalytic Converter

Catalytic converters purify emissions from gasoline and diesel engines by forcing the exhaust gas through a ceramic structure (substrate) that is coated with a precious metal catalyst, typically platinum. For gasoline engines, CO is converted to CO_2 and NO_x to nitrogen and oxygen. Volatile organic compounds are also burned forming CO_2 and water. For diesel engines, catalytic converters are primarily used to treat the NO_x compounds.

The nature of the flow in a catalytic converter is very important. By using CFD in the design of these devices, engineers can visualize and analyze physical and chemical processes associated with cold flow, light-off, and chemical reactions. Key design criteria such as flow uniformity across the substrate to maximize use of the catalyst can be easily quantified by using CFD. Design performance judged via special parameters defined by the automotive manufacturers such as pressure loss, eccentricity, flow uniformity, and gamma index, among others, can be used to define specific “pass/fail” criteria. A catalytic converter design will fail if any of the indices fall outside a preset range. These measurements can be easily determined using flow modeling software. Likewise, duration and transient temperature distribution of light-off, heat transfer, and conversion efficiencies can also be readily obtained using this technology.

Figure 2: a) flow distribution in a slice through the substrate shows catalyst utilization (cold flow analysis); b) transient temperature distribution of the exhaust gases and the substrate as predicted with CFD versus experimental data (light-off analysis), *Courtesy of University of Alberta*; c) species distribution on selected planes (chemical reactions analysis)





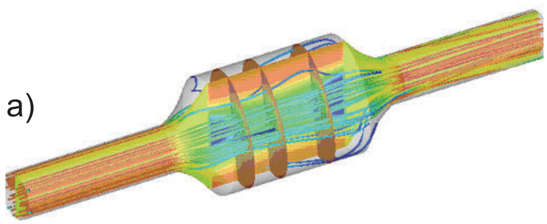
Example 2: Diesel Particulate Filter

Diesel particulate filter (DPF) is a device which removes particulate matter (by-products of incomplete combustion) from exhaust gases through physical filtration. DPF has a honeycomb structure with long parallel flow channels. Opposite ends of adjacent channels are alternatively capped, forcing gas to flow through porous side walls leaving soot behind on the surface of the walls. This process is referred to as *filter loading*. Since every filter has a finite capacity, the soot build-up must eventually be removed to prevent excessive back pressures from occurring, that would result in an adverse impact on engine performance. The cleaning process is referred to as *filter regeneration* and is typically done by rising the temperature of exhaust gases to burn off the deposit.

DPFs are typically designed around performance and durability requirements. The performance matrix includes efficient removal of particulate matter and low back pressure during loading, while durability requires that regeneration temperatures do not jeopardize the structural integrity of the filter.

CFD can be a useful tool in designing for both performance and durability targets. Using this tool, an engineer can analyze filter utilization (soot distribution in the filter), determine pressure losses, identify peak temperatures and their locations during regeneration, and assess regeneration efficiency.

a)



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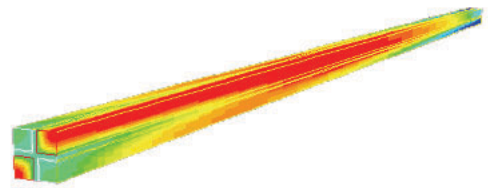

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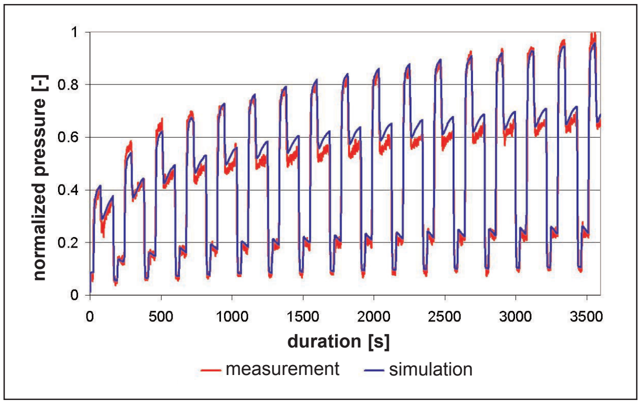


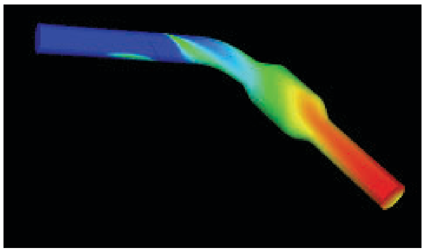
Figure 3: a) soot loading distribution; b) temperature distribution during regeneration for a single-channel; c) CFD can accurately predict pressure rise across a diesel particulate filter: experimentally measured data shown in red vs. CFD data in blue

Example 3: Selective Catalytic Reduction

Selective catalytic reduction (SCR) reduces harmful NO_x emissions through a process of chemical reactions. A water solution of urea is injected into the engine exhaust gas, leading to water evaporation and the formation of ammonia which reacts with NO_x to form nitrogen and water.

The main technical challenge with SCR is to achieve a uniform mixture of ammonia into the exhaust gas, preventing formation of local urea lean and rich conditions. The former leads to inefficient NO_x removal, while the later results in exhausting excessive, harmful ammonia through the vehicle tailpipe. The optimal mixing level removes all NO_x, while leaving no excess ammonia behind.

Since injection is inherently a three-dimensional physical process, it lends itself naturally to the benefits of CFD analyses. With CFD, an engineer can obtain very detailed information about the characteristics of both injected liquid spray and the surrounding exhaust gas, and analyze the mixing process to obtain quantitative data of the mass distribution of evaporative species.



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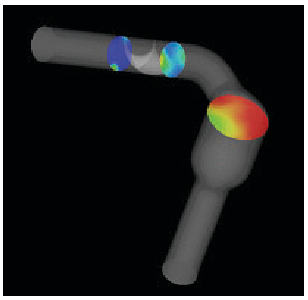

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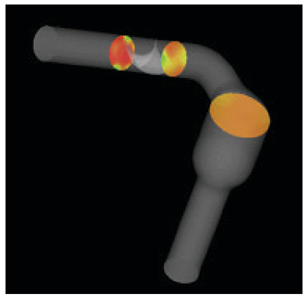

c)

Figure 4: Urea (a-b) and temperature (c) distribution for selected plane cuts reveal the level of mixing and evaporation at a specific instance in time

Example 4: Carbon Canister

Carbon canister devices are part of the evaporative emission control system. As such, they are commonly used to control the emissions of volatile hydrocarbons produced during filling of a fuel tank (so called *refueling emission*) and during vehicle operation (*evaporative emission*). The canister is filled with carbon pellets which absorb fuel vapor generated in the system, thus preventing it from escaping into the atmosphere. The hydrocarbons are then burned off by purging the canister into the intake manifold when the engine is running.

An optimum canister design includes a high working capacity, causes minimal pressure drop in the evaporative emissions system, and meets space and size restrictions, as well as the mandated emission standards. Furthermore, the carbon utilization in the canister should be uniform; when less carbon material is needed, savings are realized. In today's competitive market, carbon canister manufacturers need to cut time out of the cycle by predicting performance without having to build and test various physical prototypes.

Using CFD, quantitative performance criteria such as loading pressure drop, working capacity, and breakthrough can readily be obtained for multiple design variations of the canister geometry and various carbon pellets. In addition, local carbon utilization can be assessed through visualization of the flow feature details. CFD can help guide optimization of the canister design to reduce pressure drop and enhance carbon utilization, as well as develop more efficient devices that meet rigorous emission standards such as Ultra Low Emission Vehicle (ULEV), Super Ultra-Low Emission Vehicle (SULEV), and Partial Zero Emission Vehicle (PZEV) standards.

a)

b)

c)

Figure 5 at right: (a) pathlines show a dead zone in the upper left corner in the first of the three carbon-filled chambers; the presence of dead zones points to under-utilization of carbon; (b-c) contours of butane mass fraction on a slice through the canister during loading (left) and once the canister has reached capacity (right)
Courtesy of Expert Corporation

Conclusions

Combustion by-products from conventionally powered motor vehicles are harmful to the environment and human health, and as such have been subject to legislative regulations in US since the late 1950s. As the emission standards continue to get progressively stricter, auto manufacturers have been accelerating development of alternative powertrain technologies. Although multiple alternatives seem to hold promise for the future, further engineering developments will be needed to turn these technologies mainstream. In the near term, the fastest way to meet emission standards is to rapidly implement design improvements to key emission control devices within the conventional fleet. CFD, a proven CAE technology with broad application across the motor vehicle industry, plays an important role in the development of engineering improvements within emissions devices for conventional vehicle engines. These improvements are helping to address the near term needs of the industry to meet emission standards and to mitigate the negative effects emissions have on the environment and human health.

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[10] JD Power and Associates study, April 2006

[11] http://wardsautoworld.com/ar/auto_fueling_optimism/

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