

# Optimisation Development of Advanced Exhaust Gas After-treatment Systems for Automotive Applications

Manuel Presti, Lorenzo Pace  
Emitec GmbH

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## ABSTRACT

Future emission legislation can be met through substantial improvement in the effectiveness of the exhaust gas after-treatment system, the engine and the engine management system. For the catalytic converter, differentiation is necessary between the cold start behavior and the effectiveness at operating temperature. To be catalytically effective, a converter must be heated by the exhaust gas up to its light-off temperature. The major influential parameter for the light-off still is the supply of heat from the exhaust gas. Modification of the cold start calibration of engine control such as spark retard or increased idle speed can increase the temperature level of the exhaust gas. One further possibility is represented by a reduction of the critical mass ahead of the catalyst (exhaust manifold and pipe). Nevertheless the best measure to obtain optimal cold start effectiveness still seems to be locating the converter close to the engine. Depending on the individual application, limited installation space may only be available. Therefore the design target is a low volume, high effective catalyst with optimized thermodynamic properties to obtain maximum advantage of the thermal energy coming from the exhaust gases. The present paper deals with the cold start of a generic test cycle that can be subdivided in different phases, each characterized by different design parameters of the converter that are to be specifically tailored in order to achieve the maximum possible overall efficiency for the whole test.

## INTRODUCTION

Although car manufacturers are going through great efforts to reduce engine-out emissions (by means of optimized engine management and a/f ratio control), compliance with future emission legislation can be achieved only by aid of highly effective catalysts. As an example, assuming 2.0 gr/mi as engine-out emissions a 98% and a 99.6% HC conversion rate is required respectively for ULEV and SULEV emission limits (Fig. 1); referring to the European legislation, assuming 1.3

gr/km as engine-out emissions a 84% and a 92% HC conversion rate is required respectively for EG3 and EG4 emission limits.

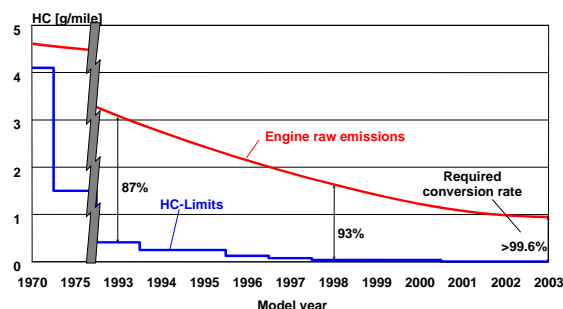


Fig. 1 – Trend of engine-out emissions, legislation limits and required conversion rates.

As a consequence physical and thermo-dynamical parameters of the entire exhaust gas after-treatment system have to be optimized and specifically tailored to each particular engine application. Matters such as catalyst substrate technology, coating technology, canning and exhaust manifold insulation belong to this procedure. Nevertheless in order to increase catalytic efficiency substrate technology still seems to offer the highest improvement potential in terms of heat capacity reduction, high temperature durability and mass transfer optimization.

## THEORETICAL AND PHYSICAL KNOW-HOW: DETERMINATION OF THE MAJOR SOURCE OF IMPROVEMENT POTENTIAL

Several factors influence in a different way the behavior of the converter. In order to find out where the major improvements can be obtained, it is useful to achieve deep insight in the degree of influence of the above mentioned parameters on system performance.

The test cycles (e.g. an ECE III Test Cycle as illustrated in Fig. 2) can be subdivided in 3 portions:

- cold start consisting of a heat sinking phase (Phase 1)

- light-off phase (Phase 1+2)
- a warm operational phase (Phase 3)

The various steps of improvements that can be achieved in emissions for the different phases of a test cycle will be discussed with aid of both experimental measurements and computer simulations

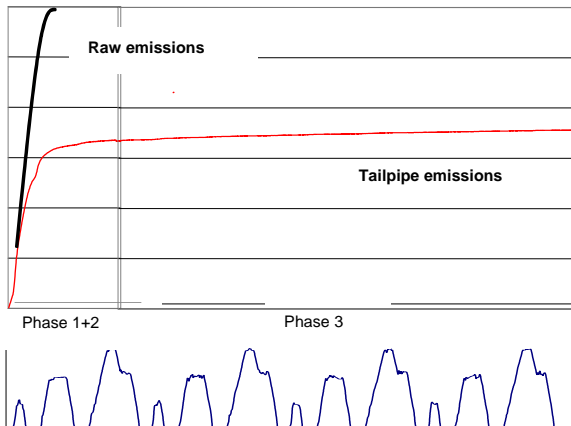


Fig. 2 – Accumulated HC-Emissions during an European Driving Cycle

Several catalysts were tested on a dynamic engine test bench simulating cold start of the FTP Cycle to investigate the influence of geometrical and physical factors on tailpipe emissions. The exhaust gas measurement was carried out modally in front of and behind the catalyst simultaneously. Moreover the gas inlet and outlet temperature were measured. All catalyst were mounted to keep the front section of the monolith at the same distance from the exhaust valves and with the same inlet cone diverging angle in order to have the same flow distribution characteristics.

#### COLD-START PHASE 1

Immediately after engine starting, the converter is heated-up by the hot exhaust gases until it reaches a light-off temperature of about 200-300 °C. During this phase the converter acts like a heat exchanger as a heat-sink device without any catalytic action. Therefore the pollutants are directly emitted into the atmosphere. In order to minimize this phase the influencing parameters of the converter are to be optimized.

The equation that describes this phase can be expressed as following:

(Eq. 1)

$$Q = \alpha \cdot GSA \cdot \Delta T$$

Where

Q= Heat flux

$\alpha$ = Heat transfer coefficient

GSA= Geometric Surface Area

$\Delta T$ = Temperature gradient between gas and wall.

The heat transfer coefficient  $\alpha$  increases with increasing exhaust gas velocity.

Therefore a way to achieve a faster light-off consists of adopting lower catalyst diameters. In

Fig. 3 it can be seen that a catalyst  $\phi$  90 mm reaches the light-off with a low mass flow at the same time as a catalyst  $\phi$  127 mm with a mass flow increased by a factor 2.

The equation that describes the „heat-exchanger behavior“ of the catalyst during the warm-up phase appears as follows:

(Eq. 2)

$$Q = m \cdot c_p \cdot \Delta T$$

where:

Q= Heat flux

m= mass of catalyst

$c_p$ = specific heat of material

$\Delta T$ = temperature increase of the substrate.

Therefore it appears clearly that in addition to the heat transfer the specific heat capacity of the substrate strongly influences the cold start behavior.

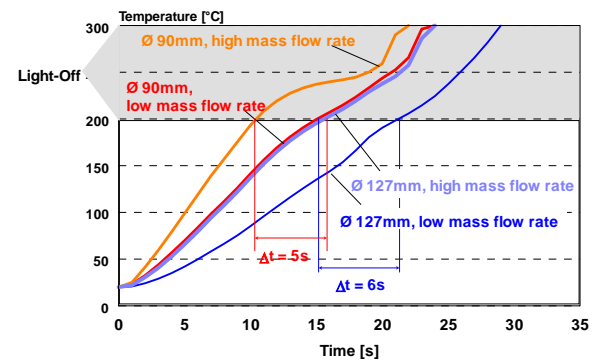


Fig. 3 – Catalyst temperature as a function of catalyst diameter and mass flow. (Substrate length 110 mm; cell density 500 cpsi)

Moreover the heat transfer coefficient increases with decreasing hydraulic diameters of the single cell. In the following table the main geometric data are listed for metallic and ceramic converters.

Converter	Hydraulic diameter [mm]	Foil- or wall-thickness [mm]
Metal 200 cpsi	1,454	0,05
Metal 400 cpsi	0,996	0,05
Metal 600 cpsi	0,85	0,04
Cer 400 cpsi	1,08	0,165
Cer 600 cpsi	0,899	0,11

Tab. 1 – Hydraulic diameters and wall thickness of different cell densities (Washcoat thickness 0.025 mm).

It appears clearly from Tab. 1 that a high cell density substrate is characterized by lower hydraulic diameters.

In Fig. 4 the temperature of substrates with different cell density is illustrated. It has to be mentioned that increasing cpsi values obviously increase substrate mass and therefore thermal inertia of the system. Therefore in order to keep the thermal mass constant it is in order to adopt thinner foils.

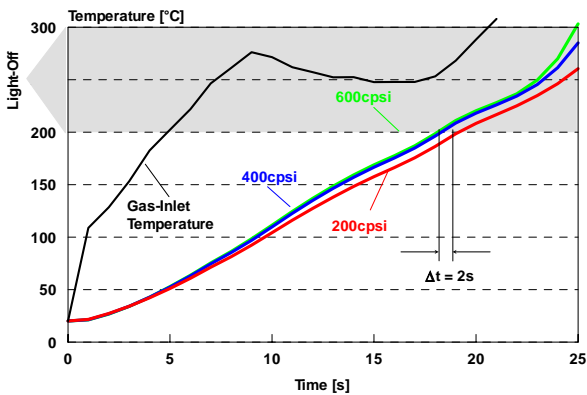


Fig. 4 - Catalyst temperature as a function of cell density. (Substrates dimensions are  $\phi$  110 x 110 mm; substrate thermal masses are constant)

The 600 cpsi converter reaches the 200 °C threshold 2 seconds earlier than the 200 cpsi catalyst.

The specific heat capacity obviously depends on substrate mass. Thinner foils allow a remarkable decrease of converter mass. The influence of foil thickness on warm-up behavior is clearly shown in Fig. 5. It can be seen that decreasing the foil thickness of about 40 % an advantage of 2.5 seconds in reaching light-off can be achieved.

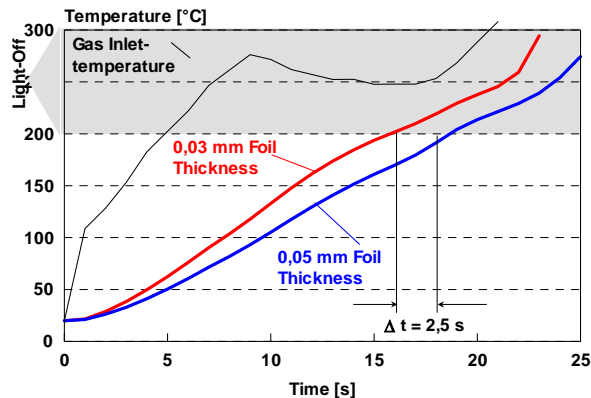


Fig. 5 – Substrate temperature 10 mm behind inlet cross section as a function of foil thickness ( $\phi$  110 x 110/500 cpsi).

Previous results [1] showed that high cpsi with the same foil thickness cause a trade-off in conversion efficiency. This is due to the fact that the influence of thermal mass increases with increasing cell density faster than the influence of GSA does (assuming a constant foil thickness). Therefore thermal inertia of the substrate 600 cpsi/50 micron foil is not compensated by its higher surface area.

The specific heat capacity of the substrate depends also on the thermal characteristics of substrate material and washcoat (Fig. 6). Moreover it can be seen that washcoat loading remarkably increases the heat capacity of the catalyst specially on low thermal mass substrates. Consequently the washcoat mass as to be kept as low as possible although ensuring a sufficient level of oxygen storage capacity.

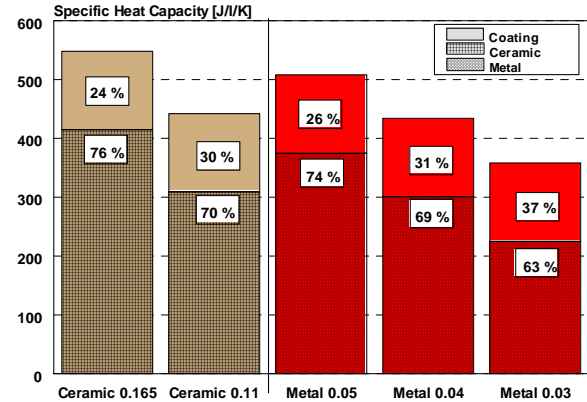


Fig. 6 – Specific heat capacity of different 400 cpsi substrates (Washcoat loading 150 g/l; T= 200 °C)

Simultaneously high cpsi values are associated with a high Geometric Surface Area (Fig. 7).

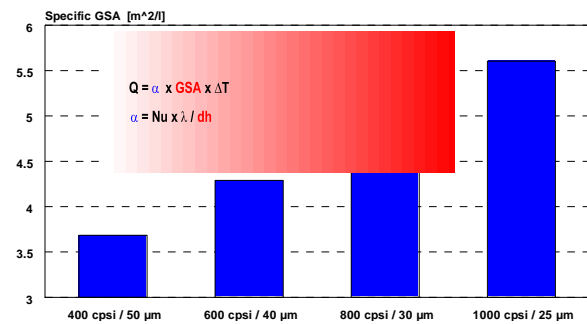


Fig. 7 – Geometric surface area values of traditional 400 cpsi converters up to newly developed high performance converters

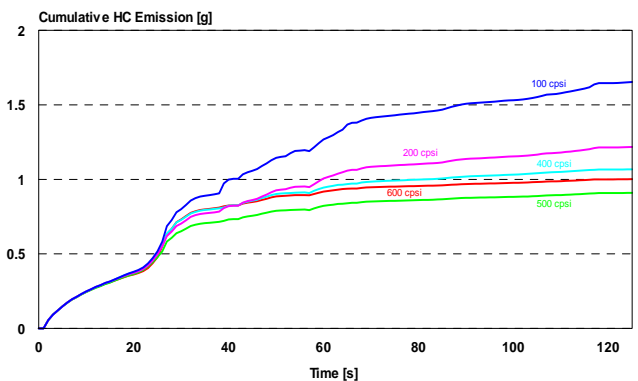


Fig. 8 – Trade-off in HC Emissions of a 600 cpsi substrate with 50 μm foil (advantage of higher surface area does not compensate the disadvantage of a higher substrate mass)

The phase 1 of cold start exerts a remarkable influence on the overall emissions of an ECE or FTP Test, since during this phase no conversion takes place. Therefore in order to obtain the maximum overall conversion efficiency for the whole test, length of phase 1 has to be reduced as much as possible.

The governing parameters of this phase can be summarized in a „Phase 1-Efficiency factor“:

$$E_1 = f(m, GSA, c_p, \phi_{id}, D)$$

Where

m= mass of substrate-washcoat

GSA= Geometric Surface Area

c<sub>p</sub>= specific heat capacity

φ<sub>id</sub>= hydraulic diameter

D= substrate diameter

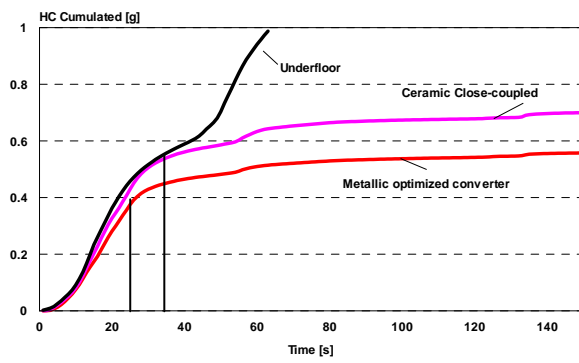


Fig. 9 – Accumulated HC-Emissions of an optimized close-coupled converter in comparison with a standard underfloor converter.

As a conclusion it can be said that adopting:

- reduced foil thickness (i.e. reduced substrate mass)
- high GSA (i.e. high cell density)
- reduced specific heat capacity
- low hydraulic diameter (i.e. high cell density)
- optimized catalyst diameter
- allows to decrease the „time-to-light-off“ of a chosen application of about 10 seconds and therefore an improvement in emissions of about 25 % (Fig. 9).

## COLD START PHASE 2

In the previous section the mechanism of warm-up behavior of the catalyst up to its light-off temperature has been explained with particular focus on the governing parameters that, once optimized, allow a remarkable improvement in emissions. In

Fig. 10 a typical light-off curve has been schematically subdivided in 3 portions. It can be seen that once a certain temperature value is reached (e.g. 220 degC) further increasing of conversion efficiency depends on the distribution of the active sites. To take the maximum advantage of the precious metals and to facilitate the diffusion of pollutant within the catalytic loading the

converter has to be coated with a thin as possible layer of washcoat.

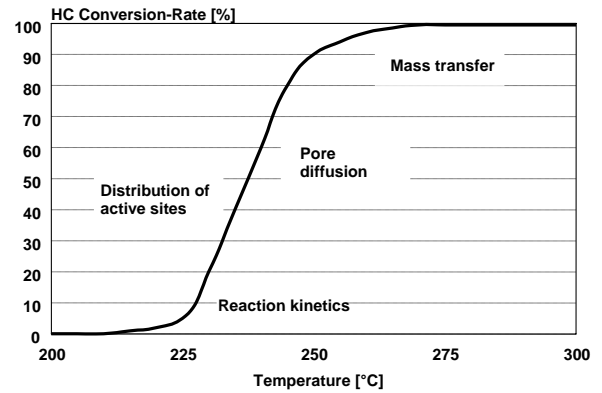


Fig. 10 – Various steps of a light-off curve with the related governing phenomena.

It can clearly be seen from Fig. 11 that increasing cell density (high GSA) enables to achieve a thinner layer of washcoat. This is due to the fact that the same washcoat mass has to be loaded upon a higher surface.

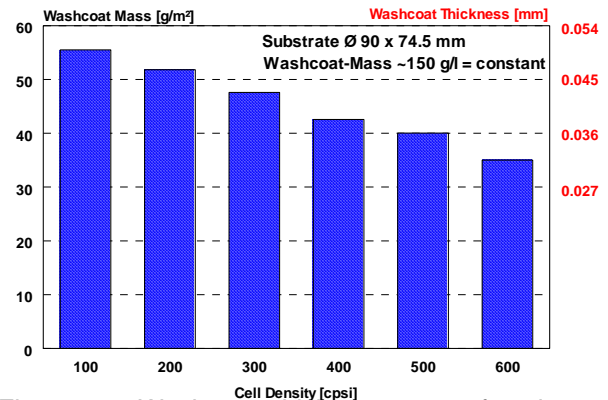


Fig. 11 – Washcoat thickness as a function of cell density

Phase 2 of cold start depends also on other parameters such as catalyst diameter. In order to illustrate this influence, the tailpipe emissions of catalytic converters with different diameters have been measured during a FTP75 Test.

It can be seen from Fig. 12 that although the converter φ 70 mm shows a better performance during the heat-sink phase (the shortest Phase 1), it becomes worse during the remaining part of cold start. This is mainly related to two reasons. The reduced inlet cross sectional area at the same catalyst length causes an excessive space velocity with short residence time of pollutants within the catalytic channels. Conversely the converter φ 127 mm shows the worse results because of the great disadvantage in phase 1.

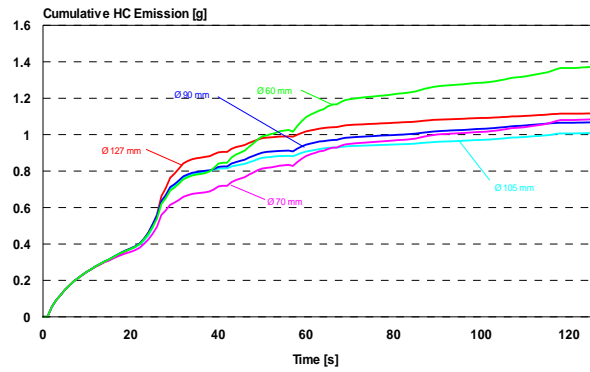


Fig. 12 – Comparison of accumulated HC-Emissions during the cold start of the FTP-Test as a function of converter diameter

In order to obtain the highest conversion potential of the catalyst, the whole substrate has to be heated above its light-off temperature. Referring to Eq. 1 and 2 it can be easily noted that a high GSA and a low  $m \cdot c_p$  values are required. In other words the GSA/specific heat capacity ratio has to be maximized. The adoption of high cell density substrate in conjunction with low foil thickness allows to fulfill this requirement (Fig. 13).

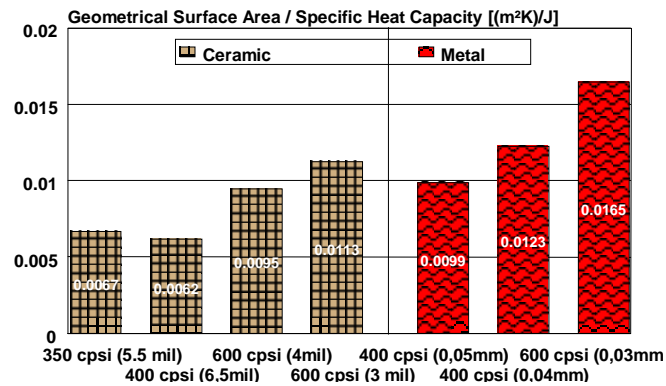


Fig. 13 – GSA/Specific Heat capacity ratio of different ceramic and metal converters.

Similarly as in previous section an efficiency factor  $E_2$  can be defined.

$$E_2 = f(\dot{m}, GSA, c_p, \phi_{id}, D, WT)$$

Where:

WT=Washcoat Thickness

$\dot{m}$  = massflow

As a conclusion the optimization of the following parameters:

- thin washcoat layer

- high GSA/specific heat ratio (i.e. high cell density and reduced foil thickness)
- low hydraulic diameter (i.e. high cell density)
- reduced engine raw-emission
- allows a remarkable improvement in tailpipe emissions (Fig. 14).

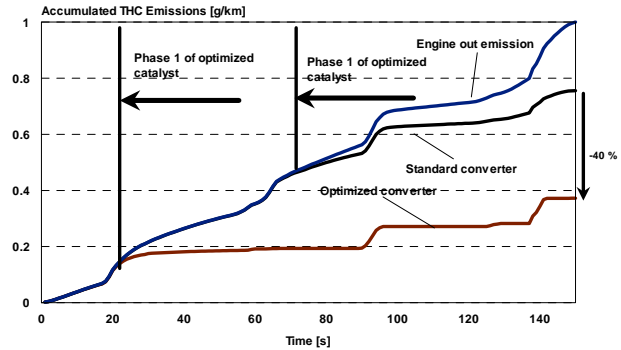


Fig. 14 – Accumulated HC-Emissions of a Phase 1+2 optimized close-coupled converter in comparison with a close-coupled converter optimized only for phase 2 in the EU Test.

### PHASE 3

As mentioned in section 1, compliance with future legislation can be achieved only by very high conversion rates during the whole test. In other words the high catalyst performance obtained during phase 1 and 2 of cold start, would be a “lost potential” if certain aspects are not considered during the warm operational phase of the test. As the most important aspects during Phase 3 the mass transfer efficiency, the oxygen storage capacity and the correct management of engine out emission are to be mentioned.

Referring to Fig. 10 it can be seen that the governing parameter of the last step to maximum catalyst effectiveness is represented by the mass transfer to channel wall. At this stage the overall conversion reaction is called “mass transfer limited“. From Fig. 15 it appears clearly that high cell density substrates are characterized by shorter diffusion paths from bulk phase to catalytic wall. Therefore low hydraulic diameter allows faster overall conversion reaction.

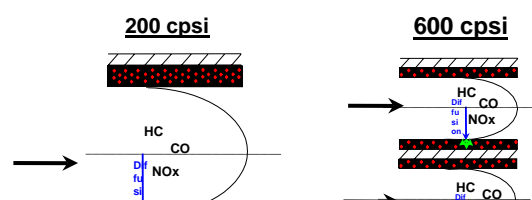


Fig. 15 – Simplified representation of the gas diffusion mechanism as a function of hydraulic diameter and cell density.

Another important factor that influences Phase 3 effectiveness is the oxygen storage capacity of the catalyst. The abounding oxygen contained in the exhaust gases during lean transients is stored in the washcoat by ceria. During rich transients the lacking O<sub>2</sub> is then “recalled” to complete the conversion reactions. The oxygen storage capacity (OSC) depends directly on washcoat mass. As explained in previous sections a remarkable improvement in cold start tailpipe emissions can be achieved by close-coupled converters with lower volume in comparison to the traditional underfloor substrates. Since the washcoat mass depends on substrate volume, close-coupled converters are characterized by lower OSC. Consequently the strategy of low volume close-coupled catalysts can be adopted only if during warm operational phase of the test a regular a/f mixture formation is ensured. By this way a constant  $\lambda=1$  value can be obtained. It has to be mentioned that the oxygen storage is mainly an adsorption mechanism and therefore it strongly depends on diffusion paths from bulk phase to channel wall. As reported in previous sections, high cell density substrates are characterized by shorter diffusion paths because of their lower hydraulic diameters and consequently by higher oxygen buffer (Tab. 2).

Cell density [cpsi]	200	300	400	500
Oxygen buffer [1/s]	1.79	2.06	2.67	2.90

Tab. 2 – Oxygen storage capacity as a function of cell density [2]

Finally it has to be said that the only way to make the above mentioned optimization measures effective consists of the correct management of engine out emissions. That means an optimized a/f ratio control that avoids high HC peaks, that would otherwise compromise both the overall effectiveness and the durability of substrate and washcoat loading.

Similarly to previous sections, an efficiency factor for Phase 3 can be defined:

$$E_3 = f(GSA, \phi_{hyd}, OSC)$$

Basing on these remarks, it appears clearly that the GSA/ hyd ratio has to be maximized. As illustrated in Fig. 16 it can be seen that increasing catalyst volume (at

constant cell density and hydraulic diameter) above a certain value does not further improve HC tailpipe emissions. This is due to the fact that GSA increases linearly with converter volume while other influencing parameters such substrate diameter remain constant). Conversely increasing cell density (with constant converter volume) allows to faster improve HC emissions.

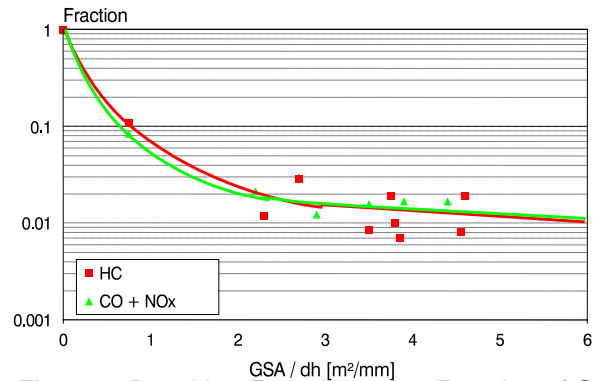


Fig. 16 – Resulting Emissions as a Function of GSA/ h (HC, CO + NOx in the EUDC Driving Cycle). [3]

As concluding remarks it can be said that by:

- high GSA
- low hydraulic diameters
- maximization of GSA/ $\phi$  hyd ratio

an improvement of HC emissions for Phase 3 of about 47 % can be achieved (Fig. 17). Moreover considering the right bar of the diagram, it can be noted that a decrease of about 80 % of emissions in comparison to a traditional underfloor converter can be achieved.

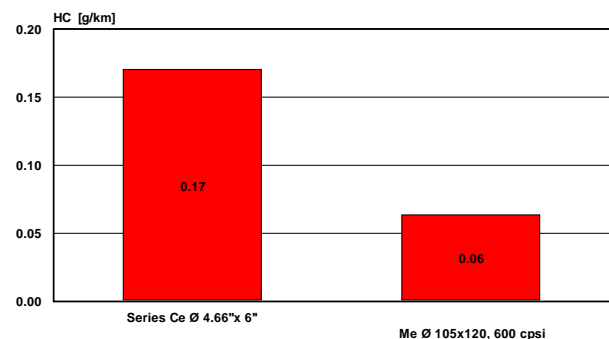


Fig. 17 – Accumulated HC tailpipe emissions of a close coupled converter with optimized parameters for Phase 3 in comparison to a standard underfloor converter.

## CONCLUSION

In the course of this work the different degrees of influence that geometrical and physical parameters of the catalyst system exert on conversion efficiency in the

various phases of a test cycle has been investigated and extensively discussed with aid of both experimental measurements (carried out on a dynamic engine test bench) and computer simulations.

The results have shown that close-coupled converters with reduced substrate volume represent the major source of improvement potential in tailpipe emissions.

It can be said that adopting:

- reduced engine raw-emission
- reduced specific heat capacity
- optimized catalyst diameter
- high GSA/specific heat ratio (i.e. high cell density and reduced foil thickness)
- thin washcoat layer
- maximization of GSA/ hyd ratio
- allows to achieve remarkable improvement in HC tailpipe emissions.

[1] Brück, R., R. Diewald, P. Hirth and F.-W. Kaiser: "Design Criteria for Metallic Substrates for Catalytic Converters", SAE Paper 950789, 1995

[2] Gottberg, I.: „Principles of the heterogenous Catalysis as in the example of the 3-way Catalytic Converter for SI-Engines“ Congress „Future Emission Legislation in Europe and USA“, Haus der Technik, Essen 1996

[3] Leveroni, E., Saroglia, G., Rossi, R.: „Catalyst Concepts for Small Volume SI-Engines: The Example of the 1.2 L Punto“, Congress „Future Emission Legislation in Europe and USA“, Haus der Technik, Essen 1996

[4] Brück, R., Maus, W.: „Motornahe Katalysatorkonzepte; Neue technische Herausforderungen“, 18 Internationales Motorensymposium, Wien 1997

[5] Pfalzgraf, B.; Rieger, M.; Ottowitz, G.: "Close-coupled Catalytic Converters for Compliance with LEV/ULEV and EG III-Legislation – Influence of Support Material, Cell Density and Mass on Emission Results", SAE-Paper 960261, 1996

[6] "New Potential Exhaust Gas Aftertreatment Technologies for "Clean Car" Legislation", Gottberg, I., Rydquist, J.E., Backlund, O., Wallman, S., Volvo Car Corporation; Maus, W., Brück, R., Swars, H., Emitec GmbH, SAE-Paper 910840

[7] Kaiser, F.-W. and S. Pelters: "Comparison of Metal Supported Catalysts with Different Cell Geometries", SAE Paper 910837, 1991

## REFERENCES