

# The Development of an Highly Modular Designed Zero-Dimensional Engine Process Calculation Code

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## ABSTRACT

The main objective of the FVV-project “Cylinder Module” was the development of a profoundly modular designed concept for object-oriented modeling of in-cylinder processes of internal combustion engines. It was designed in such a way, that it can either be used as a stand-alone real working-process calculation tool or in tools for whole vehicle simulations. It is possible to run the “Cylinder Module”-code inside the FVV-“GPA”-software for transient vehicle and driving cycle simulations and it is possible to use the graphical user interface “ATMOS” of the “GPA”-project. The code can also be used as a user-subroutine in 1-D-flow simulation codes. Much effort was spent on the requirements of flexibility and expandability in order to be well prepared to cope with the diversity of both today's and future tasks. The code is freely available for members of the German Research Association for Combustion Engines (FVV).

In the working-process calculation an analytical solution for the calculation of the difference quotients was developed, which is suitable for a user-defined number of zones in every thermodynamical system, too. As a consequence, exactly the same source code can be used for one-, two- or multi-zone calculations. In fact, additional zones can be switched on simply in case of need. It is possible to simulate a user-defined number of connected thermodynamical systems contemporaneously.

## INTRODUCTION

Without doubt, the simulation of processes inside the combustion engine plays a decisive role for the optimization of efficiency level and emissions of the total vehicle. In the process, the demands on the simulation are constantly increasing, with respect to accuracy as well as due to new combustion processes and the use of alternative fuels. For this

purpose, combustion and combustion chamber may no longer be viewed isolated from the total system. The seamless integration of the simulation of the “cylinder” in the gas exchange simulation and finally the simulation of the entire vehicle are of decisive importance, particularly for the optimization of transient processes.

To implement further advances in emissions and fuel consumption, it is necessary to be able to make statements about the behavior of the total powertrain and the vehicle at an early stage of the development. Until now, the internal combustion engine has generally been represented via characteristic maps within the simulation of the total powertrain. While this procedure ensures sufficiently short simulation times of the total model, it necessarily neglects quick changes of the boundary conditions (e.g. the gas exchange) like those occurring in transient operation. It is precisely this point which presents a future focus of the total process analysis since improvements of the emission and fuel consumption behavior of internal combustion engines are increasingly achieved by using electronic controls and controllers. For this reason, knowledge of the transient behavior of the total system at an early development stage is desirable. However, this requires the availability of a “module” in the total process analysis that represents the thermodynamic conditions in the cylinder exploded by crank angle and also takes quick changes of the boundary conditions into consideration.

This type of module can be represented in form of a zero-dimensional or quasi-dimensional real working-process calculation. While such process calculation programs are now state of the art, they generally lack modularity. The current state of engine development shows that different combustion and charge cycle procedures must be investigated with respect to their fitness for a further reduction of the emissions and efficiency increase. To represent these different

procedures within a working-process calculation, a significant development effort is generally required for the existing programs, if the structure of the software allows the necessary extensions after all (e.g. for 6 or 8-stroke procedure). For this reason, a new, fully modular, “component-style” approach for the process calculation is necessary to be able to easily integrate submodels that describe future combustion and gas exchange procedures. This was implemented in the project “FVV cylinder module” of the German Research Association for Combustion Engines (FVV).

At the same time, a large number of submodels from previous FVV research-projects were integrated in this new “Cylinder module” process calculation software (combustion, knocking, emissions, ...). [Table 1](#) provides an overview of the models already contained in the cylinder module. Until now, these submodels have been independently executable at best, but could not be combined; however, they were frequently available as non-independent executable source code which, at first, had to be adopted into a (in-house) process calculation. Until now, this has been a problem when using FVV findings in the field. FVV members often lacked the time to import source texts from research projects into an in-house process calculation.

The “cylinder module” with all its submodels from previous FVV projects offers the advantage that it is available as open source text as well as complete executable program. Future FVV model developments will also be integrated into the “cylinder module” so that they will always be available in the future as open source text and as complete executable program under this “FVV basic process calculation”. This makes them very easy to use and, at the same, they can be combined at random with models from other projects.

**Table 1. Overview of the models already contained in the FVV cylinder module**

|                                                                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                  |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| „Zylindermodul“ solver for <ul style="list-style-type: none"> <li>any number of thermodynamic systems</li> <li>any number of thermodynamic zones</li> </ul>                                                                                                                                                                                |                                                                                                                                                                                                                                                                  |
| new caloric approach for any fuels (burned and unburned)<br>conventional approaches for calorics (Justi, de Jaegher, Zacharias, ...)                                                                                                                                                                                                       |                                                                                                                                                                                                                                                                  |
| Combustion: <ul style="list-style-type: none"> <li>Wiebe</li> <li>import from file</li> <li>Barba burn rate</li> <li>empirical Barba-model (CI)</li> <li>entrainment-model (hom. SI)</li> <li>Witt approach (hom. SI)</li> <li>quasidim. Auer approach (CNG, with / without prechamber)</li> <li>Hoppe approach (stratified SI)</li> </ul> | Initial values according to Zapf<br>FVV approach for internal residual gas return<br>Heat transfer: <ul style="list-style-type: none"> <li>Woschni / Woschni-Huber</li> <li>Hohenberg</li> <li>Bargende</li> <li>interface „FVV-Wandtemperaturmodell“</li> </ul> |
| Other: <ul style="list-style-type: none"> <li>fuel injection (SI/CI)</li> <li>fuel evaporation</li> <li>knock: Franzke</li> <li>knock: Worret</li> <li>turbulence</li> </ul>                                                                                                                                                               | Emissions: <ul style="list-style-type: none"> <li>Zeldovich</li> <li>Kořuch (NO, CI)</li> <li>Heider (NO, CI)</li> <li>Hohlbaum (NO, CI)</li> </ul>                                                                                                              |
| gas exchange (fill and empty method)                                                                                                                                                                                                                                                                                                       |                                                                                                                                                                                                                                                                  |

## OVERVIEW

The “FVV cylinder module” can be used in the following variants:

- As independent simulation software with a gas exchange simulation based on the “fill and empty” method with any number of containers.
- As independent simulation software that limits itself to the simulation of the high-pressure part of the working process. This is an important procedure particularly for investigating the combustion. In this case, the boundary conditions at inlet valve close must be set. This can be done either by means of measuring data or they can be calculated using the “Zapf” approximation approach or with the help of the “FVV residual exhaust gas model”.
- As Matlab extension (“DLL” or “mex32”), optionally with or without charge-exchange calculation, see [Figure 1](#). Applications: e.g. the “cylinder module” as precise “heat source” of the engine in a thermal management model of the total vehicle (Simulink). Or generally for automated calculations and optimizations.
- As “cylinder module” in the “GPA” software. This FVV-owned program can also be used to perform total system views. Until now, the cylinder or combustion could only be set there as characteristic map. Now, the “cylinder module” can be used which responds to changes of the boundary conditions, thereby allowing meaningful transient simulations, see [Figure 2](#). Of interest: In the GPA software, the “cylinder module” can also be combined with the engine wall temperature model of the FVV (e.g. cold start).

<[figure 1](#) here>

<[figure 2](#) here>

The “cylinder module” source code is designed so that it is relatively easy to integrate it in 1-D fluid dynamics software on principle where it can replace the high-pressure calculation part of the cylinder objects.

This flexible integration possibility of the cylinder module in all types of different “simulation environments” was an important requirement during the development. The central requirement of the draft of a “future-quality process calculation” lead to the selection of an object-oriented basic structure for the simulation source code, among other things. In this object-oriented basic structure, submodels can be replaced and added at random. It is possible to compute using any number of “thermodynamic systems”, the submodels can be combined with any type of system and can also communicate among each other or couple with each other.

Previous process calculation codes supported either only a single or two-zone calculation or even a multi-zone

calculation, which would then have to be solved iteratively [13]. In the framework of the FVV “cylinder module” project, an analytical solution of this problem was developed that can compute as “n-zone” with any number of zones. By selecting “n = 1” or “n = 2”, the code can also work as single or two zone. Based on the analytical formulation, the n-zone solver does not feature any disadvantage with respect to speed compared to an explicit single or two-zone solver. But at the same time, it offers the flexibility, particularly in model development, to be able to activate additional zones at any time. Compared to an iterative solution of a multi-zone problem that has been customary until now, the analytical solver offers enormous advantages with respect to speed.

In current process computing programs, the known models from Justi [10], Zacharias [15] and de Jaegher [2] are generally to represent the properties of the working gas. They represent the required caloric variables, such as the individual gas constant, the specific inner energy and its partial derivatives. These models were each developed for a certain fuel composition and can be applied to new, alternative fuels, such as E85, natural gas or hydrogen, only to a delimited extent - or not at all. For this reason, a caloric approach for freely definable fuels was developed in the framework of the “cylinder module” project.

The typical computing time for a working cycle with two zones without charge exchange is between 300 ms and 3 seconds on a standard PC. A calculation with charge exchange simulation requires about 10 to 30 seconds on a standard PC.

## OBJECT-ORIENTED PROCESS CALCULATION

Figure 3 shows an example for a simulation with gas exchange according to the fill and empty method with four thermodynamic systems. “System 1” is the combustion chamber with variable volume (piston movement) and it is modeled as two-zone. “System 2” represents the intake system. This can be modeled as 1-zone or 2-zone; for a 2-zone representation, residual gas flowing back from the combustion chamber is stored in a separated zone. The two outlet containers are calculated as single zone systems 3 and 4.

“Simulation modules” can now be integrated into every system. A Wiebe combustion, for example, is a “simulation module”. The Wiebe combustion is typically linked with the “combustion chamber” system. However, it is irrelevant to the cylinder module solver - any “simulation module” can be linked with any system. This makes the cylinder module very flexible. Just a short time ago, it would have been difficult to image that a combustion could take place in an outlet container. Now, such a configuration in the context of exhaust gas aftertreatment is justified. Or: For a prechamber

engine, the combustion can also act in the independent “prechamber” system. And: At the same time, the “Wiebe combustion” simulation module can also be “integrated” three times: Once for the actual combustion chamber, once for the outlet container and once for a prechamber. This simulation module is then activated in three “instances”, each instance calculates independently and is parameterized differently for the corresponding specific application.

But back to Figure 3 showing the charge-exchange calculation as an example. This figure depicts six instances of the “throttle equation” simulation module. The leakage (blow-by) flows via “throttle equation A” past the piston rings into the crankcase, which is represented as a “virtual system” with constant pressure and constant temperature. Intake and exhaust valve respond via “throttle equation C” and “throttle equation D” whose flow cross-section  $A_{eff}$  is controlled on a time variable basis by valve modules. This “valve” simulation modules are coupled internally with the corresponding “throttle equation” simulation module and provide the time-variable flow cross-section  $A_{eff}$  depending on time, valve stroke and flow coefficients. If  $A_{eff}$  equals zero, the valve is closed. Intake and outlet containers are also connected with the environment (“virtual system”) or among each other (between “system 3” and “4”) via “throttle equations”.

In summary: The cylinder module solver can solve the thermodynamic basic equations for any number of systems and zones. The cylinder module consists of a large number of “simulation modules”. The user decides which simulation modules should be “activated”, and on which systems and zones they should act or with which other simulation modules they should “communicate”. It is also possible to integrate or “activate” simulation modules multiple times, i.e. in several instances.

<figure 3 here>

## CALORICS FOR ANY FUEL

Process calculation uses two central equations of thermodynamics: The instantaneous energy balance (first law of thermodynamics) and the thermal state equation of the working gas. These two equations are required in differential form for process calculation.

First law of thermodynamics:

$$\frac{dQ}{d\varphi} + \frac{dH}{d\varphi} - p \cdot \frac{dV}{d\varphi} = u \cdot \frac{dm}{d\varphi} + m \cdot \left( \frac{\partial u}{\partial T} \cdot \frac{dT}{d\varphi} + \frac{\partial u}{\partial p} \cdot \frac{dp}{d\varphi} + \frac{\partial u}{\partial \lambda} \cdot \frac{d\lambda}{d\varphi} \right) \quad (1)$$

Thermal state equation:

$$p \cdot \frac{dV}{d\phi} + V \cdot \frac{dp}{d\phi} = m \cdot \frac{dR}{d\phi} + \frac{dm}{d\phi} \cdot R \cdot T + m \cdot T \cdot \left( \frac{\partial R}{\partial T} \cdot \frac{dT}{d\phi} + \frac{\partial R}{\partial p} \cdot \frac{dp}{d\phi} + \frac{\partial R}{\partial \lambda} \cdot \frac{d\lambda}{d\phi} \right) \quad (2)$$

The caloric material properties of the working gas refer in the following to the specific internal energy, the specific enthalpy and the individual gas constant, as well as the partial derivatives of these three variables. These caloric properties are shaded gray in [equations \(1\) and \(2\)](#). The number of marked variables informally leads to this: Without knowledge of these caloric properties, no meaningful process calculation is possible.

So far, these variables were generally calculated using the approaches of Justi [10], Zacharias [15] or de Jaegher [2]. Each of these models were, however, developed for a specific fuel composition and can be applied to new, alternative fuels only to a limited extent - or not at all. Since the importance of alternative fuels will undoubtedly increase, a new calorics approach was also developed in the framework of the FVV "cylinder module" project.

Creating a truly universal calorics for any type of fuel was a great scientific challenge. Since the calculation foundations have already been published several times ([9], [5], [6]), the focus below will be on the application of the new approach.

In calorics, a distinction must be made between the burned gas calorics, which is responsible for burned gas (exhaust gas and returned residual gas) and air, and the calorics for unburned fuel vapor.

## BURNED GAS CALORICS

The new burned gas calorics of the "cylinder module" was developed for freely definable fuels. The fuel is defined via its C/H/O/N atomic ratio. An equilibrium calculation is performed for the respective fuel, the current temperature, pressure and air ratio. It provides the concentrations of the most important chemical species in the combustion chamber. The dissociation, i.e. the breakdown of molecules into radicals at high temperatures and, therefore, the real gas behavior, are also represented. The calorics of the gas mixture is then calculated via a "component approach" from the concentrations and properties of the individual species.

Previous component approaches for burned gas calorics mostly work "offline": Equilibrium calculation and component approach were performed for a matrix of temperatures, pressures and air ratios. The results were saved as a table. The actual working process calculation then loaded this table and interpolated in it. A new, heavily, optimized

procedure for determining the equilibrium concentrations was used in the FVV cylinder module. It offers enormous speed advantages compared to a classic Newton procedure and is approximately 50 times faster. In this way, an "online" calculation of the caloric properties without a speed disadvantage now becomes practically possible. And: The new approach is suitable for any type of fuel.

The intermolecular interactions were not taken into account. Such effects must be considered only if the temperature is lower than 1.5 times the "critical temperature" and the pressure reaches at least 0.5 times the "critical pressure". These "critical" areas, including the listed safety factors for CO<sub>2</sub> and H<sub>2</sub>O, have been included in [Figure 4](#), all other components are negligible. The "critical" combination of very low temperatures and high pressures can practically not be achieved in the combustion chamber, the closest approximation occur at high supercharging with external exhaust-gas recirculation and strong charge-air cooling. A present-day commercial vehicle engine, which is operated at high EGR rates even under full load, serves as an example in the following. [Figure 4](#) shows the compression graph of a commercial vehicle full load point with 30% EGR that runs at a clear distance to the areas in which intermolecular interactions must be considered. The figure also shows a compression graph with 0% EGR. By increasing the compression ratio, the "critical area" could be reached, but it would once again be unproblematic since there would be no significant H<sub>2</sub>O concentration in the combustion chamber during the compression without EGR.

The new calorics approach is first integrated into the "cylinder module" process calculation. For purposes of comparison or backward compatibility, it is also possible to select the approaches according to Justi, Zacharias or de Jaegher. If the cylinder module calorics is to be integrated into another simulation software, it can also be done without any problems. The source text is available with detailed documented interfaces as Fortran code. An integration into C/C++ is also possible via the corresponding and included interfaces.

In addition, a Matlab interface of the cylinder module calorics is available which allows the caloric properties or equilibrium concentrations to be calculated quickly and conveniently from within Matlab.