

A holistic model-based simulation of fuel supply systems for alternative fuels

David van Bebber *, Heiko Baum** and Werner Willems *

Ford Research and Innovation Center Aachen, Susterfeldstraße 200, 52072 Aachen, Germany*

FLUIDON GmbH, Jülicher Straße 338a, 52070 Aachen, Germany**

E-Mail: dvanbebber@ford.com, heiko.baum@fluidon.com

For compression ignition engines, dimethyl ether (DME, $\text{CH}_3\text{-O-CH}_3$) has been studied as a promising renewable synthetic fuel candidate to replace Diesel fuel. However, since DME is gaseous at ambient pressure the use of DME poses special challenges for the design of the new fuel systems. Therefore, a holistic model-based approach is required to support vehicle specific DME fuel supply system adaptations. The paper presents a thermo-hydraulic system simulation model of a generalized DME fuel supply system to explain the fundamental simulation capabilities.

Keywords: thermal-hydraulic simulation, holistic system analysis, model-based system development, parallelization of 1D-system simulation, dimethyl ether (DME)

Target audience: Mobile Hydraulics, Mining Industry, Design Process

1 Introduction

Synthetic fuels from renewable energy sources have and are being studied for their potential to reduce greenhouse gas emissions from internal combustion engines. DME (dimethyl ether = $\text{CH}_3\text{-O-CH}_3$) has been shown to be a suitable substitute fuel for diesel. Already in 2010 Yanai et al. [1] published a paper about the optimization of injection pressure for fuel consumption and exhaust emissions reduction in a dimethyl ether (DME) engine with a common rail type injection system. The recent "xME-Diesel" project [2] confirmed that a conversion to DME fuel is possible with available high-pressure components. However, the use of DME also poses special challenges for the design of the fuel supply system, which is especially caused by fuel property differences between DME and Diesel.

1.1 What is DME

The DME fact sheet from North Carolina State University gives a fundamental introduction to what DME is [3]: "DME stands for Dimethyl Ether. It is a clean burning, energy efficient, renewable fuel, and an alternative choice to Diesel. ... DME is a simple ether, an isomer of ethanol and an aerosol propellant. As a propellant, it has been used in a variety of spray cans. ... Its application as a fuel for trucks, however, has led many to call it the 'fuel of the future'. ... DME can be produced from many sources like biomass, waste products, agricultural products, natural gas and coal. The most popular way of producing DME is by methanol dehydration."

1.2 Challenges to a DME capable fuel supply system

Besides the combustion advantages, there are also a few disadvantages for the application of DME. A quote from a report of Advanced Biofuels USA states [4]: "DME is not a 'drop-in' fuel like renewable diesel. Although DME has a high cetane number and does not require spark plugs, high pressure, or cryogenics like CNG and LNG, its differences in density, viscosity, lubricity, etc., require a DME fuel system (renewable or fossil-based) with different fuel injectors to allow higher flow. It also requires a different fuel pump and fuel storage tank although it has fewer requirements for after-treatment equipment. To maintain a liquid state, DME requires around 73 psi or 5 bars of pressure, less pressure than required to liquefy propane such as that used in a barbecue grill."

Figure 1 shows a comparison of the fluid properties of DME and of Diesel [1] as well as a 3D-visualization that illustrates the enormous density change between DME at liquid and gaseous phase along the vapor pressure curve.

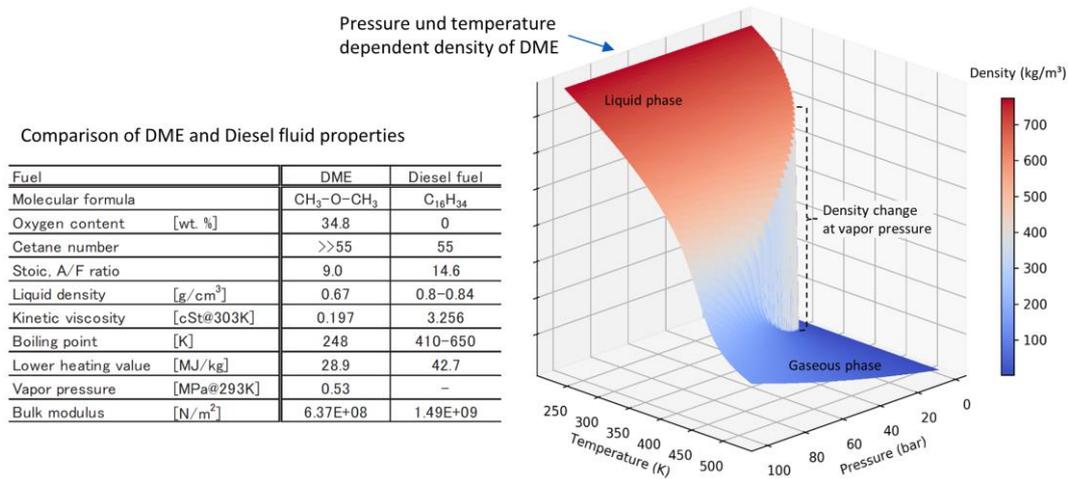


Figure 1: Fluid properties of DME and Diesel [1] and DME density versus temperature and pressure

From Yanai's report [1] it gets clear that a common rail fuel system conversion from diesel to DME requires multiple system adjustment to maintain a satisfying system performance from the combustion and injection supply system point of view. Regarding the global fuel system, it is comprehensible that adjustments to individual components will have dynamic effects on neighboring components. Of particular interest, for the functional reliability of the fuel supply system, is the thermal balance of the low-pressure circuit.

The following two examples outline the range of impacts that must be considered when designing a DME fuel supply system or retrofitting an existing diesel fuel supply system.

- Low-pressure fuel supply system heats up during long waiting times with hot engine (loading, unloading, refueling, etc.). This is caused on the one hand by leakages in the high-pressure components and on the other hand by the heat transfer through the fuel lines installed in the engine compartment. The resulting temperature rise of the DME has a direct influence on the pressure in the low-pressure side of the fuel supply system. Although the tank and lines are usually pressure-resistant up to over 30 bar, problems can still arise for the operation of the fuel supply system. For example, it is not guaranteed that a refueling system can fill the vehicle at the increased pressure. One consequence of this is, for example, the need for a forced heat transfer via cooling elements or an active cooling.
- Due to the required higher volume flow through the underfloor lines, compared to diesel fuel supply systems, pressure losses due to hydraulic resistances can cause the pressure on the suction side of the boost pump to fall locally below the vapor pressure of DME, which results in the formation of vapor bubbles. This endangers the proper functioning of this pump, which is positioned between the prefill pump of the tank and the high-pressure pump (HDP) at the engine. The task of the boost pump is to maintain the pressure on the suction side of the high-pressure pump (HDP) at approx. 30 bar so that vapor bubbles cannot form in the suction tract of the HDP under any circumstances.

The three examples illustrate the challenges of a low-pressure fuel system suitable for DME, whether for a new development or as a conversion kit for a vehicle in the existing fleet. The general design of such a system and also the control of the cooling system requires an in-depth understanding of the system which is difficult to obtain only by road and dynamometer tests. Since each low-pressure DME fuel supply system must be individually adapted to the vehicle, a holistic fuel system development by means of a 0D/1D dynamic system simulation is highly desired and in case of the high-pressure side of the fuel supply system industry standard. In this context **Figure 2** presents a representative configuration of a common rail based DME fuel system that shall act as a reference

configuration for the subsequently introduced simulation model. The color coding of the fuel lines indicates that the DME fuel system has three instead of two (diesel) different pressure levels.

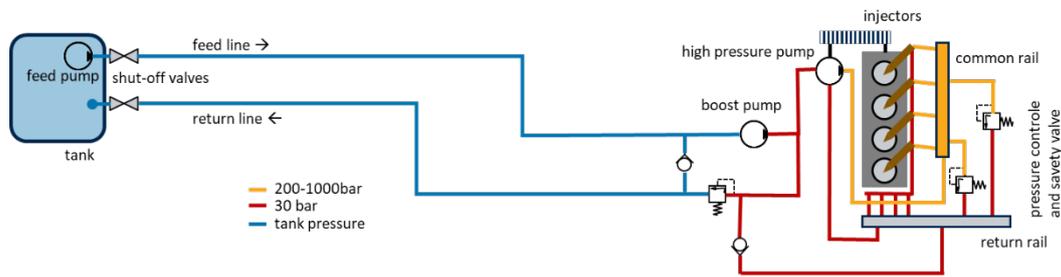


Figure 2: Configuration of a generic DME fuel supply system

2 Generic DME fuel supply system simulation model

A holistic view of the DME fuel supply system is realized in a model-based system development environment including thermo-hydraulic sub-models (DSH $plus$ [5]). To obtain meaningful simulation results, the following key aspects of modeling are considered in the simulation approach:

- Pipe model with thermo-hydraulic calculation and with transport equation for variable gas content
- Consideration of different environmental temperatures along the system's fuel lines
- Resistance description with consideration of gas and steam cavitation

2.1 Extended distributed parameter MOC pipe model

Pipe models based on method of characteristic (MOC)[6][7] are already proved to be able to obtain accurate simulation results for highly dynamic injection systems in a short computation time [8].

In the last years the fundamental MOC algorithm was extended with features like thermo-hydraulic, vapor and gas cavitation as well as gas transport, which are mandatory for a DME injection system simulation. **Figure 3** summarizes the current functionalities that are implemented in the used MOC pipe model.

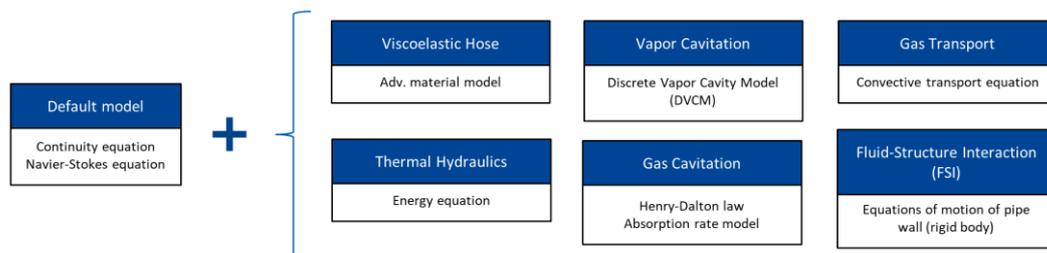


Figure 3: MOC pipe model [5]

The governing model equations vary depending on the analysis target. For the DME system simulation the following pipe model options are utilized:

- Default model: These equations are always solved to evaluate the system's dynamic.
- Thermal hydraulics: Heat transfer through pipe walls and dissipative heating due to pressure losses.
- Mixed Cavitation and gas transport, pressure- and temperature dependent development of undissolved gas and its travel with the fluid.

2.1.1 Mixed cavitation in a DME fuel system

Since no liquid is free of entrapped gas, there is always some dissolved and undissolved gas present in the liquid. To simplify the 1D simulation, a homogenous mixture of fuel and gas is assumed. In addition, a transport of

dissolved and undissolved gas with fluid velocity is presumed (no slip). **Figure 4** shows the basic model assumption of mixed cavitation in a DME fuel system.

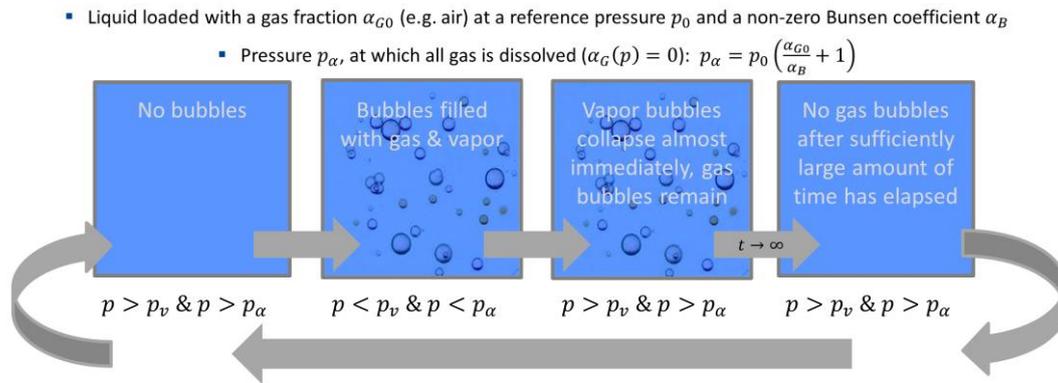


Figure 4: Mixed cavitation: vapor and gas cavitation

In a first step, a situation such as after a long standstill of the vehicle, the complete gas is dissolved in the fluid and no gas bubbles exist. In this context α_{G0} represents the total volume fraction of the gas at standard conditions. However, the liquid's capability to dissolve gas decreases with decreasing pressure. According to Henry's Law, the volume fraction of the undissolved gas $\alpha_G(p)$ is proportional to the pressure p and the Bunsen coefficient α_B [9]. Hence, gas is released if the pressure drops below the pressure p_α at which all gas is dissolved. This phenomenon is referred to as *gas cavitation*. *Vapor cavitation* occurs if the fuel pressure drops below the vapor pressure $p_v(T)$. The vapor bubbles collapse immediately after the pressure again exceeds the vapor pressure $p_v(T)$. However, the originally dissolved gas released by the liquid converted into vapor remains as undissolved gas. In many situations, a *mixed type* of cavitation occurs where bubbles are created which are filled with vapor and gas [10]. Desorption of gas during gas cavitation as well as absorption of the gas subsequent to a cavitation event does not happen instantaneously. Especially absorption does take considerable time, which results in a propagation of gas bubbles into the downstream system, due to the fluid flow. As a common approximation to cover this effect, a PT_1 behavior is used. The necessary time constants T_{Abs} and T_{Des} for absorption and desorption must be measured or estimated. Thus, the gas bubbles are slowly dissipated due to Henry's law and the specific time constant. When the pressure exceeds p_α , the gas bubbles disappear as a function of the absorption time constant.

2.1.2 Combined MOC interpolation methods for coping with a variable sonic velocity of the fluid

Besides the fact, that any form of cavitation does have unfavorable and unwanted effects onto the system dynamic performance (noise, reduced efficiency), the resulting undissolved air has an influence onto the propagation speed of information in the fluid, which must be considered to design a pressure oscillation free fuel supply system.

The propagation speed of information in a pipe ($\lambda_i = c \pm v_{flow}$) depends on the current speed of sound c and the liquid velocity v_{flow} . The liquid velocity in typical fuel supply systems is much smaller than the speed of sound. Thus, the propagation speed mainly depends on the speed of sound.

In case of a nearly constant speed of sound (with or without consideration of undissolved gas) the classical spatial interpolation method, such as explained in [6][7], can be used for the MOC scheme. According to the Courant-Friedrichs-Lewy criteria ($CFL = \lambda \Delta t / \Delta x$) the pipe is subdivided into a 1D numerical grid. The spatial interpolation scheme is stable for $CFL \leq 1$ (**Figure 5**, left side).

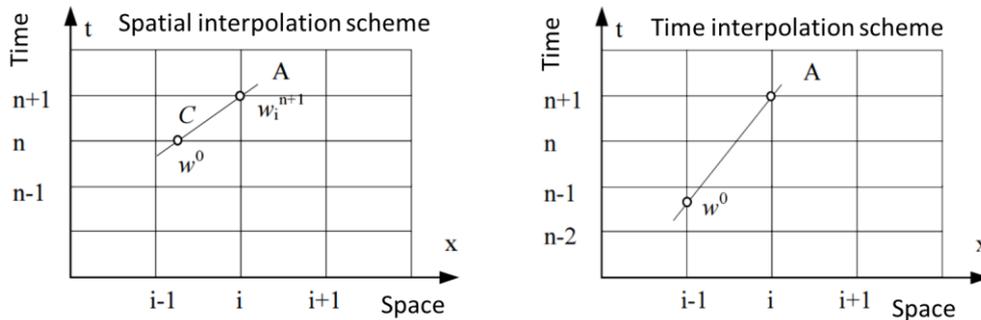


Figure 5: Time and spatial interpolation as described in [11]

Due to the high vapor pressure of DME, short-term gas bubbles in the liquid cannot be avoided, which consequently changes the speed of sound and thus the propagation speed of information. In order to cover the changes in the propagation speed of information and thus the change in the CFL condition, but at the same time avoid reinitialization of the numerical grid, an additional time interpolation is used (Figure 5, right side), as introduced by [11]. The time-line interpolation is applied in cavitation-free regions with low propagation speeds and guarantees low numerical damping even with unfavorable CFL numbers. Unfortunately, this interpolation is only applicable for nearly constant propagation speed. Thus, in transitional regions the conventional spatial interpolation must be used.

2.1.3 Position specific heat transfer

The thermal behavior of the fuel system is of particular interest for the functional reliability of the injection system. Therefore, the default MOC momentum and continuity equation system is expanded by the energy equation. The implemented mathematical model, which is not shown in detail, covers the following effects:

- Heat transfer between the fluid and the environment (description by thermal transmittance)
- Dissipative heating due to the friction related pressure drop along pipe
- Change of pressure due to a change of the fluid's temperature (closed system)
- The transport of energy with the flow (convective transport)

The mathematical model currently does not take the following effects into account:

- Enhancement of heat transfer due to unsteady flow
- Pressure, flow rate or temperature-dependent heat transfer coefficients
- Thermal conduction in axial direction
- Thermal capacity of the pipe wall

Figure 6 briefly explains how the heat flow at each internal grid point of the MOC pipe model is calculated.

The thermal transmittance U between the liquid and the environment is calculated:

$$U = \frac{1}{\frac{1}{\alpha_i} + \frac{r_i}{k_W} \ln\left(\frac{r_a}{r_i}\right) + \frac{r_i}{\alpha_a r_a}}$$

The heat flux \dot{q}'' (per unit area of the inner pipe surface) exchanged between liquid and environment is then given by:

$$\dot{q}'' = U(T_F - T_{Env})$$

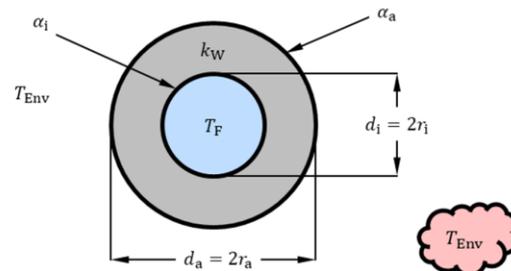


Figure 6: Heat flow calculation of the MOC pipe model [5]

Internal and external heat transfer coefficients (α_i, α_a), thermal conductivity of pipe material (k_w), and pipe wall thickness ($r_a - r_i$) are component parameters. To consider changing environmental temperature conditions, it is possible to apply a look-up table for an environmental temperature T_{Env} distribution along the pipe. Transient environmental temperature situations are enabled by the option to assign a variable external heat transfer coefficient or heat flux.

2.2 Resistor with consideration of gas and vapor cavitation

DME fuel supply systems have several resistors that not only create pressure differences along the flow path. Through a phenomenon that is called choked flow, resistors can also affect the volume fraction of undissolved gas downstream of the resistor. Of specific interest is the situation at which the static pressure in the vena contracta of the resistor falls below vapor pressure and vapor cavitation occurs, generating bubbles that contain both DME vapor and undissolved gas. The result is a condition that limits the flow rate through the resistor (Figure 7, left hand side).

As the bubbles move down stream, the flow velocity decreases and the static pressure rises. This causes the vapor fraction of the bubbles to condense abruptly, creating unwanted noise and shock waves that can damage components. The remaining fraction of undissolved gas migrates further downstream with the flow, potentially causing problems due to altered fluid properties. Although noise and shock wave effects are not covered by the present 1D simulation, the simulation still can support design efforts to avoid choked flow situations.

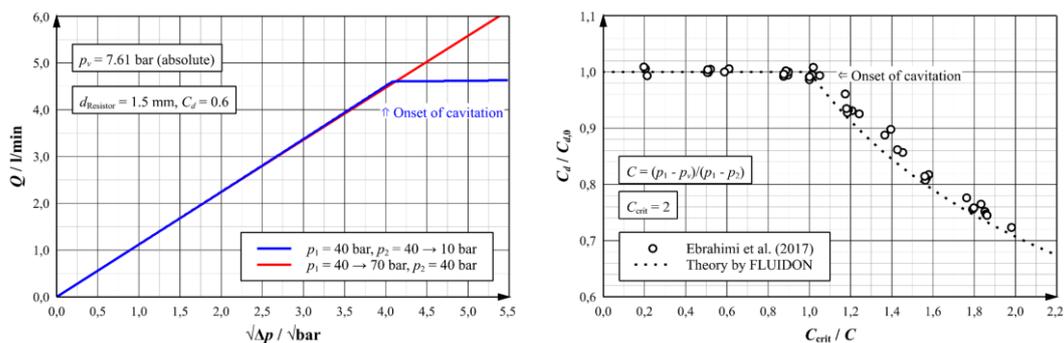


Figure 7: Pressure and bubbles along resistor

The two examples in the left-hand graphic of Figure 7 illustrate that the occurrence of cavitation depends not only on the pressure difference at the resistor, but mainly on the pressure on the downstream side of the resistor. Given the high vapor pressure of DME (see Figure 1), which increases the risk of flow choking, an accurate representation of choked flow within the resistor model is therefore essential for a realistic simulation of the DME fuel system. The right-hand graphic of Figure 7 presents a validation of the criteria that determines the onset of cavitation and is included in the resistor component model, using published measurements of choked flow.

2.3 DME fuel supply simulation model

The final generic fuel supply system simulation model is shown in Figure 8. The model is used to check the basic functionality of all sub-models and the fundamental system behavior. The model is a simplification of the real vehicle fuel system and only used for qualitative tests. Therefore, the injectors are reduced to their fixed internal hydraulic channel geometry or even simplified to a single pipe resistor combination. To shorten the simulation time in the first tests, the feed and return lines are reduced from ~5 m to 1 m length.

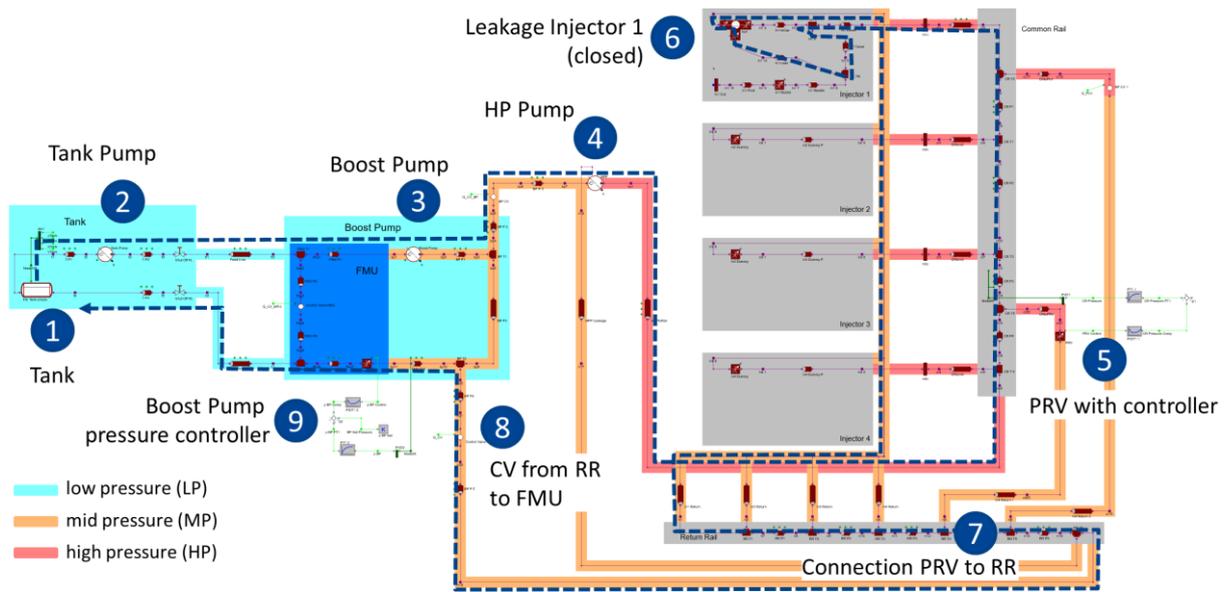


Figure 8: Simulation model of fuel supply and injection system

The initial conditions of the simulation are set to:

- Pressure levels
 - Tank: 7 bar
 - Boost pump and return rail: 30 bar
 - Common rail: 50 bar
- Temperatures
 - Fluid and environment: 300 K
 - Engine compartment: 370 K (common rail and return rail)
 - Heat Transfer for all surfaces of the high pressure and return rail components is set to $50 \frac{W}{m^2K}$,
low pressure fuel lines to $15 \frac{W}{m^2K}$.

To achieve a smooth simulation start, the tank pump starts first. Afterwards, the boost pump ramps-up and subsequently the high-pressure pump starts, which raises the common rail pressure from 50 to 900 bar. Injection starts after 5 s.

To provide an overview of the complex thermo-hydraulic situation within a DME fuel supply system, a simulation result snapshot at 10 s (Figure 9) shall be briefly discussed along the numbers flow path shown in Figure 8.

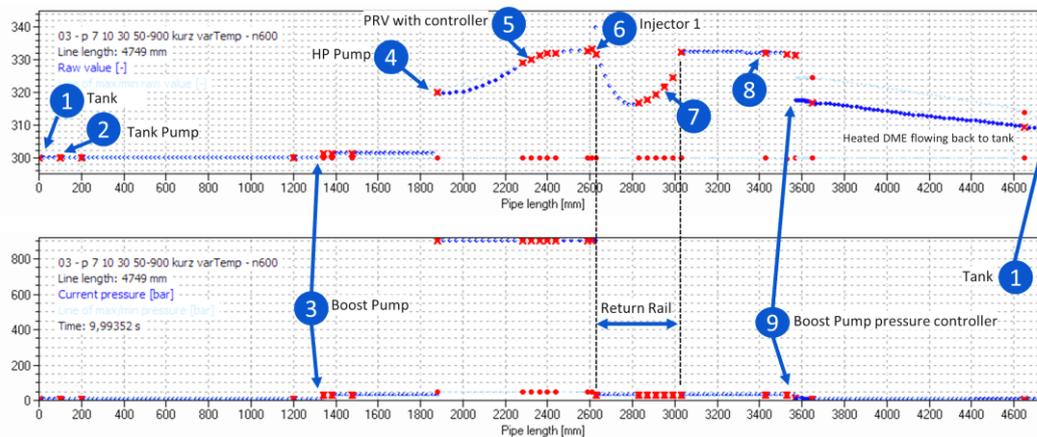


Figure 9: Simulation results along selected pipe circuit after $t = 10$ s (temperature and pressure)

The feed pump (2) conveys the fluid from the tank (1) to the boost pump (3), which increases the pressure at the suction side of the high-pressure pump (4) to 30 bar before the high-pressure pump finally increases the pressure to 900 bar. At each pump, the temperature rises corresponding to the achieved pressure difference. High-pressure pump, common rail (5) and injector (6) feature the same pressure. Although the pressure at the high-pressure pump, the common rail and the injectors are at the same level, there is a continuous increase in temperature along the path, which is caused by the heat transfer from the engine compartment into the pipes. The fuel in the injector return line is still colder and heats up only slowly by the small leakage flow and the temperature in the engine compartment (**Figure 10**). The pressure of the leakage flow naturally falls to the mean pressure level. The connected return rail (7) already shows an additional heat-up due to the four injectors leakage flows as well as some return flow from the pressure control valve. The significantly higher temperature at the end of the return rail is caused by the hot leakage return flow from the high-pressure pump. At the boost pump pressure control valve (9), some fuel of the mid pressure level flows into the return line. The return line heats up slowly but is also cooled by the environment. The shortened return line is not long enough to fully cool down the fuel, which will be different with the original return line length of 5 meter. At the end, the return flow is mixed with the tank fuel and the cycle restarts.

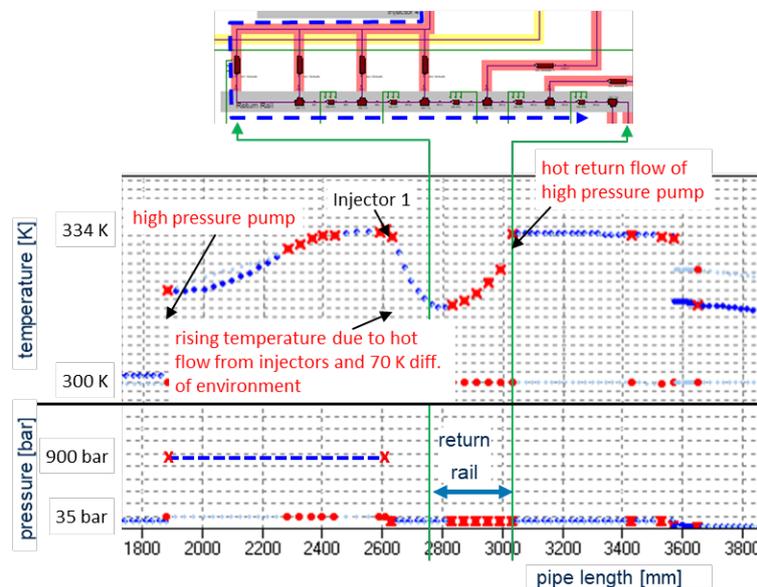


Figure 10: Zoom view onto the injector return line ($t = 10$ s, temperature and pressure)

3 Acceleration of the system simulation by parallelization of the pipe calculation

The brief discussion of the snapshot of the simulation result at 10 s already gives an impression of how complex the thermo-hydraulic situation in a DME fuel supply system is. To evaluate a full system duty cycle to determine lack of dynamic performance or the occurrence of pressure oscillation problems, long simulation times that meet real-world use cases must be evaluated and numerous parameter configurations must be analyzed. To achieve these goals in a practicable time frame, intra-model parallelization of the pipe calculation and parallel batch simulation on a Linux server are used. The model of the DME fuel supply system consists of 48 tubes with large differences in the length of the pipes. Due to the CFL criteria, this leads to an individual discretization of the pipes, which means a different computational load for each of the pipes. In such a situation simply parallelizing all 48 pipes would not be beneficial, since short (faster) pipes must wait until long (slower) pipes have completed their calculation. Moreover, parallelization of simulation models requires some overhead on computational effort to start the parallel calculations and consolidate the results. For systems with many short pipes, this can lead to so much numerical overhead that hardly any computing time is saved. In order to achieve a maximum out of parallelization at a minimum overhead, the pipes are grouped (pooled). **Figure 11** introduces possible load balanced distributions of the pipes of the DME fuel supply system simulation model. Each colored block represents

a separate pipe with its own number of elements (block height). The horizontal line shows the optimum number of elements for each pool with equal distribution.

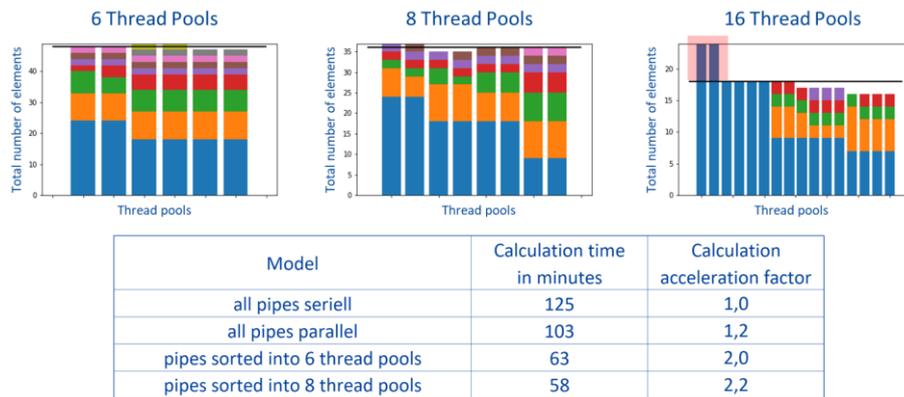


Figure 11: Possible thread pool distribution of the pipes of the simulation model

Even if the results in Figure 11 look simple, sorting pipes automatically into thread pools is not a trivial task. A bin packing algorithm [12] had to be applied to setup the thread pool configurations. As can be seen in Figure 11 configurations with 6 and 8 pools are possible for the DME fuel supply system simulation model. Whereas a configuration with 16 thread pools would not give further improvement, because two of the pipes have to many grid elements and would better be subdivided in two shorter pipes. The result table in Figure 11 summarizes the realized simulation times. As expected, a parallelization of all pipes does not gain much reduction of simulation time. Whereas for the given example the two load balanced thread pools are able to reduce the simulation time by a factor of two.

4 Use of the generic simulation model of the DME fuel system.

To make the best use of the now numerically optimized DME fuel supply system simulation model, the model is implemented into a simulation workflow. **Figure 12** presents the virtual engineering lab (VEL) environment, that is used to host the simulation workflow.

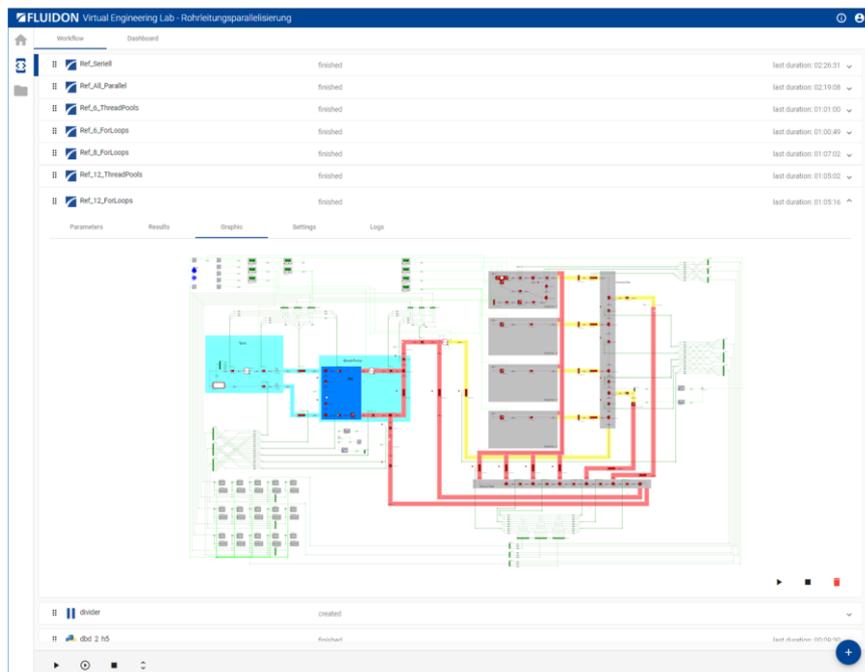


Figure 12: DME fuel supply system simulation model on the VEL

As presented in [13] the VEL is not only able to run simulation models but also to run python script jobs for pre- and post-processing, which automatically create a PowerPoint report of the analyzed simulation results.

With the DME fuel supply system simulation model now driven by a simulation workflow, the designer can fully focus on the design objective and use dynamic thermal-hydraulic system simulation as the design tool it was intended to be. Time-consuming activities such as the setup of the next simulation study or the subsequent preparation of results for discussions with customers/colleagues are pushed into the background. The designer can fully concentrate on the analysis of his results and use the workflow e.g. for the investigations [14][15][16].

5 Summary and Outlook

The paper introduced DME as a potential renewable substitute for conventional diesel fuels. However, to realize this, a vehicle-specific design of the DME fuel supply system is required, regardless of whether the development focus is on a new vehicle or retrofitting an existing vehicle. Due to the complex thermo-hydraulic situation within the DME fuel supply system, a holistic model-based development approach is required. The generalized DME fuel supply system simulation model, introduced in this paper, is the right tool to perform the necessary design studies. Embedded into a simulation workflow, the simulation model serves the development engineer as a tool that largely automates the generates information (virtual measurement data) that would otherwise only be available after time-consuming test bench trials. Conceptual decisions can thus be made much earlier in the development process, thanks to an improved data basis.

Nomenclature

<i>Variable</i>	<i>Description</i>	<i>Unit</i>
p_F	Surface Pressure	[bar]
T	Temperature	[K]
α_i	Heat transfer coefficients	[W/(m ² *K)]
k_w	Thermal conductivity	[W/(m*K)]
CFL	Courant-Friedrichs-Lewy-Zahl $c = \frac{u\Delta t}{\Delta x}$	[]
u	speed	[m/s]
x	distance	[m]
t	time	[s]
λ	propagation speed	[m/s]
n	time step	[]
i	cell number	[]
T	time constant	[s]
p	pressure	[bar]
\dot{q}	heat flux	[W/m ²]
r	radius	[m]
c	speed of sound	[m/s]
v	flow speed	[m/s]

References

- [1] Yanai, T., et al., *Optimization Of Injection Pressure For Fuel Consumption And Exhaust Emissions In A Dimethyl Ether (Dme) Engine With A Common Rail Type Injection System*, Journal of KONES Powertrain and Transport, Vol. 17, No. 2, Page 519 – 532, 2010
- [2] Willems, W., et al., *xME-Diesel – (Bio-)Methyl Ether as an Alternative Fuel for Bivalent Diesel Combustion*, 6th TMFB Conference Tailor-Made Fuels, Page 77 – 79, 2018
- [3] n., n., *DME fact sheet*, North Carolina State University, Campus Box 7409, Raleigh, NC 27695 | 919-515-3480 | www.nccleantech.ncsu.edu | , 2016
- [4] n., n., *What's the Difference between Biodiesel and Renewable (Green) Diesel? - or - What Renewable Fuels Can Be Used in Compression Ignition Engines?* Advanced Biofuels USA, Page 30-31, 2020
- [5] n. n.; „DSHplus – Simulationsprogramm für fluidtechnisch mechatronische Systeme“, www.fluidon.com, FLUIDON Gesellschaft für Fluidtechnik mbH, Aachen, 2022
- [6] Theissen, H.: *Die Berücksichtigung instationärer Rohrströmung bei der Simulation hydraulischer Anlagen*, Dissertation, RWTH Aachen, 1983
- [7] Müller, B., *Einsatz der Simulation zur Pulsations- und Geräuschkinderung hydraulischer Anlagen*, Dissertation RWTH Aachen, 2002
- [8] van Bebber, D; “*Reduction of Pressure Waves in Common Rail Systems by Improving System Design Parameters*”. Conference Proceedings, 5. International Fluid Power Conference – IFK. Aachen, Germany, 2006
- [9] Wikipedia contributors, "Henry's law," *Wikipedia, The Free Encyclopedia*, https://en.wikipedia.org/w/index.php?title=Henry%27s_law (accessed February 12, 2022), 2022
- [10] Baum, H., Scheffel, G.; *Disordered flow to the reservoir – measures to improve the situation*, Proceedings of the 11th International Fluid Power Conference (11. IFK), Volume 3, Page 437-447, 2018
- [11] Šavar, M., Virag, Z., Kobbar, R.: *A variant of the method of characteristics for hyperbolic conservation laws*. In: VIIIth international conference Numerical methods in continuum mechanics, 2000
- [12] Wikipedia contributors, "Bin packing problem," *Wikipedia, The Free Encyclopedia*, https://en.wikipedia.org/w/index.php?title=Bin_packing_problem (accessed February 15, 2022), 2022
- [13] Baum, H., Müller, B., Breuer, O., „*Die Orchestrirung digitaler Zwillinge für Industrie 4.0*“, 8. Fachtagung hybride und energieeffiziente Antriebe für mobile Arbeitsmaschinen, Karlsruhe, Seiten 133 - 146, ISBN 978-3-7315-1071-0, 2021
- [14] Baum, H., Eibl, S., Merk, J., *Pressure Oscillation Analysis in Low-pressure Fuel Piping Systems*, MTZ worldwide, Page 60-65, 2017
- [15] Baum, H., Pasquini, E., *Druckschwingungsanalyse in Kraftstoffversorgungsanlagen - 11. Tagung Einspritzung und Kraftstoffe*, Page 337-358, 2018
- [16] Baum, H., *Druckschwingungsanalyse hydrostatischer Antriebsstränge - O+ P Fluidtechnik*, Band 63, Ausgabe 6, Page 36-41, 2019