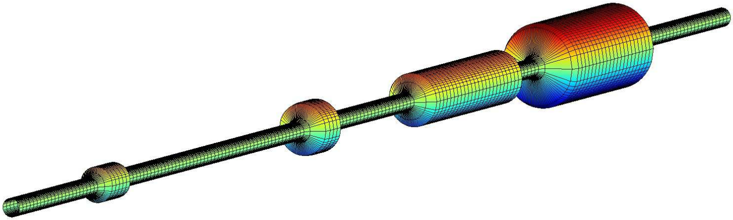
Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Martin Rybicki, Universität Hamburg

Modeling, Simulation and Optimization of Gas Dynamics in an Exhaust Pipe: A Network Approach



June 28, 2012

Agenda

1. Motivation
2. Modeling
3. Network
4. Numerical simulation
5. Optimization
6. Conclusion

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

1 Motivation
2 Modeling
3 Network
4 Numerical simulation
5 Optimization
6 Conclusion

Exhaust gas pollution

Figure: exhaust gas emission[1] and air pollution in China[2]

[1] http://www.thedailygreen.com/cm/thedailygreen/images/o6/car-exhaust-lg.jpg
[2] http://climatechange.foreignpolicyblogs.com/files/2010/09/china-air-pollution.jpg

Catalytic converter

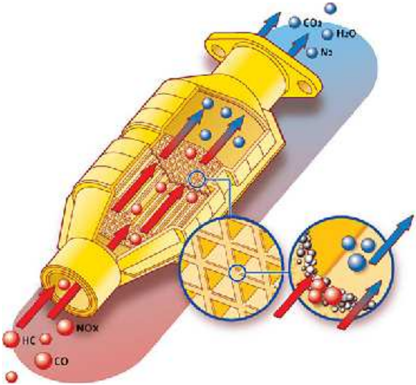


Figure: catalytic converter[3]

- Catalytic converters reduces needed activation energy for the transformation of harmful gases into less harmful gases
- Honeycomb structure provides a large reaction surface
- Reaction only happens when activation energy $\tilde{E}^+ \approx 600K$ is reached ("light off")

[3] http://www.timbarkerstudio.com/technical/catalytic_converter.jpg

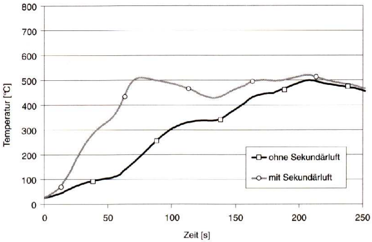
Catalytic converter II

How to ensure sufficient high temperatures in the catalytic converter just after the engine start?

- Choose λ-ratio less than 1.

$$\lambda = \frac{m_{air}}{m_{air}^{st}}$$

- Unburnt gas is transported to the catalytic converter, where it reacts exothermically
- Required oxygen is given by a pump



R. van Basshuysen and F. Schäfer Handbuch Verbrennungsmotor Vieweg 2005 ,page 711

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

1 Motivation
2 Modeling
3 Network
4 Numerical simulation
5 Optimization
6 Conclusion

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Modeling

- Gas flow through a pipe with a variable duct
- physical effects have to be included, such as
  - wall friction
  - heat transfer through the wall
  - combustion in the catalytic converters
  - friction in the catalytic converters due to honeycomb structure

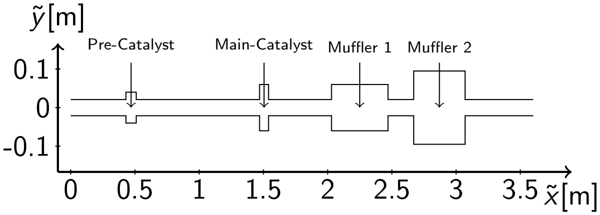


Figure: Geometry of the exhaust pipe

First model

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

$$
\begin{aligned}
(\tilde{A}\tilde{\rho})_{\tilde{t}} + (\tilde{A}\tilde{\rho}\tilde{u})_{\tilde{x}} =& 0 \\
(\tilde{A}\tilde{\rho}\tilde{u})_{\tilde{t}} + (\tilde{A}\tilde{\rho}\tilde{u}^2)_{\tilde{x}} + \tilde{A}\tilde{p}_{\tilde{x}} =& -\frac{\xi}{4}\pi\tilde{d}\tilde{\rho}\frac{\tilde{u}^2}{2} - \tilde{C}_c\tilde{A}\tilde{\chi}\tilde{\rho}\tilde{u} \\
(\tilde{A}\tilde{\rho}\tilde{E})_{\tilde{t}} + (\tilde{A}\tilde{\rho}\tilde{u}\tilde{E} + \tilde{A}\tilde{u}\tilde{p})_{\tilde{x}} =& -\tilde{h}\pi\tilde{d}(\tilde{T} - \tilde{T}_{\text{Wall}}) \\
& + \tilde{q}_0\tilde{A}\tilde{\chi}\tilde{\rho}\tilde{z}\tilde{K}(\tilde{T}) \\
(\tilde{A}\tilde{\rho}\tilde{z})_{\tilde{t}} + (\tilde{A}\tilde{\rho}\tilde{u}\tilde{z})_{\tilde{x}} =& -\tilde{A}\tilde{\chi}\tilde{\rho}\tilde{z}\tilde{K}(\tilde{T}) \\
\tilde{p} =& R\tilde{\rho}\tilde{T}
\end{aligned}
\tag{1}
$$

with $\tilde{E} = c_v\tilde{T} + \frac{\tilde{u}^2}{2}$, $\tilde{K}(\tilde{T}) := \tilde{K}_0 \cdot \exp(-\tilde{E}^+/\tilde{T})$ (*Arrhenius' law*) and $\tilde{\chi}(x) = 1 \Leftrightarrow x$ is in one of the two catalytic converters, and vanishes otherwise.

R. Natalini and L. Lacoste for MAGNETTI MARELLI
Mathematical modeling of chemical processes in exhaust pipe
Technical Report, IAC Rome, 2004.

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

New model

Model for a network of single pipes.

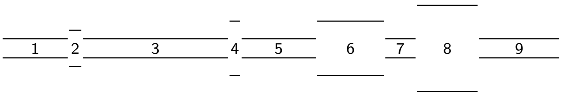


Figure: Network of 9 connected pipes

Use model (**??**) with constant cross section to derive a model for the single pipes.

New model II

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Model for a single pipe with diameter $\tilde{d}$ containing a catalytic converter.

$$
\begin{aligned}
\tilde{\rho}_{\tilde{t}} + (\tilde{\rho}\tilde{u})_{\tilde{x}} &= 0 \\
(\tilde{\rho}\tilde{u})_{\tilde{t}} + (\tilde{\rho}\tilde{u}^2 + \tilde{p})_{\tilde{x}} &= -\frac{\xi}{\tilde{d}}\tilde{\rho}\frac{\tilde{u}^2}{2} - \tilde{C}_c\tilde{\rho}\tilde{u} \\
(\tilde{\rho}\tilde{E})_{\tilde{t}} + (\tilde{\rho}\tilde{u}\tilde{E} + \tilde{u}\tilde{p})_{\tilde{x}} &= -\frac{4\tilde{h}}{\tilde{d}}(\tilde{T} - \tilde{T}_{\text{Wall}}) + \tilde{q}_0\tilde{\rho}\tilde{z}\tilde{K}(\tilde{T}) \\
(\tilde{\rho}\tilde{z})_{\tilde{t}} + (\tilde{\rho}\tilde{u}\tilde{z})_{\tilde{x}} &= -\tilde{\rho}\tilde{z}\tilde{K}(\tilde{T}) \\
\tilde{p} &= R\tilde{\rho}\tilde{T}
\end{aligned}
\tag{2}
$$

New model II

Model for a single pipe with diameter $\tilde{d}$ containing a catalytic converter.

$$\begin{aligned} \tilde{\rho}_{\tilde{t}} + (\tilde{\rho}\tilde{u})_{\tilde{x}} &= 0 \\ (\tilde{\rho}\tilde{u})_{\tilde{t}} + (\tilde{\rho}\tilde{u}^2 + \tilde{p})_{\tilde{x}} &= -\frac{\xi}{\tilde{d}}\tilde{\rho}\frac{\tilde{u}^2}{2} - \tilde{C}_c\tilde{\rho}\tilde{u} \\ (\tilde{\rho}\tilde{E})_{\tilde{t}} + (\tilde{\rho}\tilde{u}\tilde{E} + \tilde{u}\tilde{p})_{\tilde{x}} &= -\frac{4\tilde{h}}{\tilde{d}}(\tilde{T} - \tilde{T}_{\text{Wall}}) + \tilde{q}_0\tilde{\rho}\tilde{z}\tilde{K}(\tilde{T}) \\ (\tilde{\rho}\tilde{z})_{\tilde{t}} + (\tilde{\rho}\tilde{u}\tilde{z})_{\tilde{x}} &= -\tilde{\rho}\tilde{z}\tilde{K}(\tilde{T}) \\ \tilde{p} &= R\tilde{\rho}\tilde{T} \end{aligned} \tag{2}$$

Simplify this model:

1. Scale
2. Small Mach number $\rightarrow$ asymptotic model

Scaling

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Replace each quantity ($\tilde{y}$) by the product of the reference quantity (y_r) and the dimensionless quantity (y).

Quantity	Unit	Reference quantity	Reference value
$\tilde{t}$	s	$t_r = x_r/u_r$	$0.01 - 0.093$s
$\tilde{x}$	m	$x_r = L$	$0.1 - 0.93$m
$\tilde{\rho}$	kg m^{-3}	ρ_r	1.2 kg m^{-3}
$\tilde{u}$	m s^{-1}	u_r	10 m s^{-1}
$\tilde{p}$	kg m^{-1} s^{-2}	p_r	10^5kg m^{-1} s^{-2}
$\tilde{T}$	K	$T_r = p_r/(R\rho_r)$	300 K
$\tilde{z}$		z_r	0.1

Table: Quantities, Units, Reference quantities, Reference values

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Full Euler model (FE)

Dimensionless model, full Euler model (FE)

$$
\boxed{\begin{aligned}
\rho_t + (\rho u)_x &= 0 \\
(\rho u)_t + (\rho u^2)_x + \left(\frac{1}{\gamma M^2}\right) p_x &= -C_f \rho \frac{u^2}{2} - C_c \rho u \\
(\rho T + (\gamma-1)\gamma M^2 \rho \frac{u^2}{2})_t + (\rho u T + (\gamma-1)\gamma M^2 \rho \frac{u^3}{2})_x & \\
+ (\gamma-1)(up)_x &= -h(T - T_{\text{Wall}}) + q_0 \rho z K(T) \\
(\rho z)_t + (\rho u z)_x &= -\rho z K(T) \\
p &= \rho T
\end{aligned}} \tag{FE}
$$

$$M = u_r \sqrt{\frac{\rho_r}{\gamma p_r}} \approx 3 \cdot 10^{-2}, \ \left(\frac{1}{\gamma M^2}\right) \approx 10^3, \ (\gamma - 1)\gamma M^2 \approx 4.8 \cdot 10^{-4}$$

Asymptotic model (AM)

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Asymptotic expansion in $\varepsilon = \gamma M^2$ in the quantities, i.e.

$$p(x,t) = p_0(x) + \varepsilon p_1(x,t) + \mathcal{O}(\varepsilon^2)$$

leads to an asymptotic model.

Asymptotic model (AM)

Asymptotic expansion in $\varepsilon = \gamma M^2$ in the quantities, i.e.

$$p(x,t) = p_0(x) + \varepsilon p_1(x,t) + \mathcal{O}(\varepsilon^2)$$

leads to an asymptotic model.

$$\boxed{\begin{aligned}
\rho_t + (v+Q)\rho_x &= -\, q\rho \\
z_t + (v+Q)z_x &= -\, zK(T) \\
v_t &= \frac{1}{\int_0^1 \rho dx}\Bigg[p_l - p_r - \int_0^1 \rho Q_t dx - \int_0^1 \rho(v+Q)q dx \\
&\quad - C_f \int_0^1 \frac{\rho(v+Q)^2}{2} dx - C_c \int_0^1 \rho(v+Q)\, dx\Bigg]
\end{aligned}}$$

(AM)

The exhaust pipe as a network

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

- Each pipe ($i = 1, \ldots, 9$) needs 4 boundary conditions (data we do not have).
- Connect 9 pipes to a network by defining **coupling conditions** at the vertices

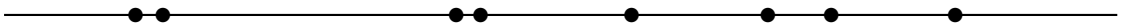


Figure: Network of 9 connected pipes and 8 vertices

Coupling conditions

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

1. Conservation of mass

$$\rho_r^{i-1} = \rho_l^i \quad \forall\ i = 2, \ldots, 9 \tag{3}$$

2. Conservation of the ratio of unburnt gas

$$z_r^{i-1} = z_l^i \quad \forall\ i = 2, \ldots, 9 \tag{4}$$

3. Conservation of internal energy (temperature)

$$u_r^{i-1} A^{i-1} = u_l^i A^i \quad \forall\ i = 2, \ldots, 9 \tag{5}$$

Coupling conditions for the pressure

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

1. First idea: Conservation of pressure at the vertices

$$p_r^i = p_V^i = p_l^{i+1} \tag{6}$$

Coupling conditions for the pressure

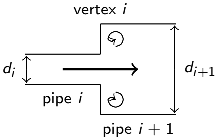
1. First idea: ~~Conservation of pressure at the vertices~~

$$p_r^i = p_V^i = p_l^{i+1} + f_{ext}^i \tag{6}$$

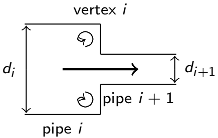
2. Include pressure loss term (*minor losses*) at the vertices.

$$f_{ext}^i = \begin{cases} \rho_r^i \dfrac{(u_r^i)^2}{2} \left(1 - \dfrac{d_i^2}{d_{i+1}^2}\right)^2 & \text{sudden expension} \\ 0.5 \cdot \rho_l^{i+1} \dfrac{(u_l^{i+1})^2}{2} \left(1 - \dfrac{d_{i+1}^2}{d_i^2}\right) & \text{sudden contraction} \end{cases}$$

sudden expansion

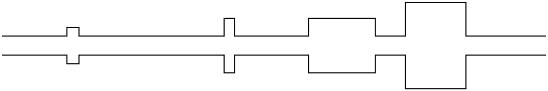


sudden contraction



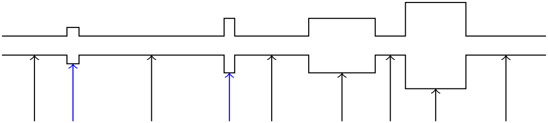
Overview

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion



Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

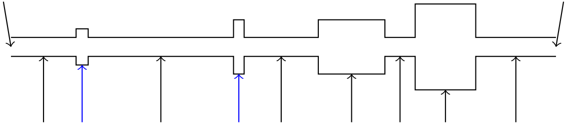
Overview



$$
\begin{aligned}
\rho_t + (v+Q)\rho_x &= -q\rho \\
z_t + (v+Q)z_x &= -zK(T) \\
v_t &= \frac{1}{\int_0^1 \rho dx}\Bigg[p_l - p_r - \int_0^1 \rho Q_t dx - \int_0^1 \rho(v+Q)q dx \\
&\quad - C_f \int_0^1 \frac{\rho(v+Q)^2}{2} dx - C_c \int_0^1 \rho(v+Q)\, dx\Bigg]
\end{aligned}
$$

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Initial (engine start) and boundary conditions



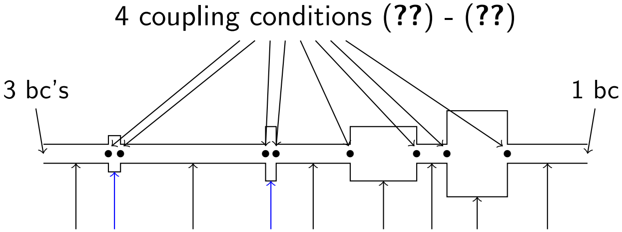
$$\rho_t + (v+Q)\rho_x = -q\rho$$

$$z_t + (v+Q)z_x = -zK(T)$$

$$v_t = \frac{1}{\int_0^1 \rho dx}\left[p_l - p_r - \int_0^1 \rho Q_t dx - \int_0^1 \rho(v+Q)q dx - C_f \int_0^1 \frac{\rho(v+Q)^2}{2} dx - C_c \int_0^1 \rho(v+Q)\, dx\right]$$

Overview

Initial (engine start) and boundary conditions



$$
\begin{aligned}
\rho_t + (v+Q)\rho_x &= -q\rho \\
z_t + (v+Q)z_x &= {\color{blue}-zK(T)} \\
v_t &= \frac{1}{\int_0^1 \rho\, dx}\Bigg[p_l - p_r - \int_0^1 \rho Q_t\, dx - \int_0^1 \rho(v+Q)q\, dx \\
&\qquad - C_f \int_0^1 \frac{\rho(v+Q)^2}{2}\, dx - {\color{blue}C_c \int_0^1 \rho(v+Q)\, dx}\Bigg]
\end{aligned}
$$

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Numerical costs

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

CFL-condition for (FE)	CFL-condition for (AM)
$\lambda_{max}\dfrac{\Delta t}{\Delta x} \leq c_N$	$u_{max}\dfrac{\Delta t}{\Delta x} \leq c_N$
with $\lambda_{max} := \max\lvert\lambda\rvert$	with $u_{max} := \max\lvert u\rvert$

c_N denotes the Courant number. $u \geq 0 \Rightarrow \lambda_{max} = u_{max} + c$, where c denotes speed of sound. Then

$$\Delta t_{AM} = \frac{\lambda_{max}}{u_{max}}\Delta t_{FE} = \left(1 + \frac{1}{M}\right)\Delta t_{FE} \tag{7}$$

Furthermore the computation of one spatial steps for the full Euler model takes approximatly 5 times as many *flops* as for the asymptotic model.

Some numerical simulations

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

We will compare the **full Euler model (??)** with the **asymptotic model (??)**.

- Single pipe
  - high pressure difference
  - low pressure difference
- Whole exhaust pipe
  - high pressure difference
  - low pressure difference
- Sensibility numerical solutions to the minor loss term

Single pipe: Example 1

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

(FE) (AM)

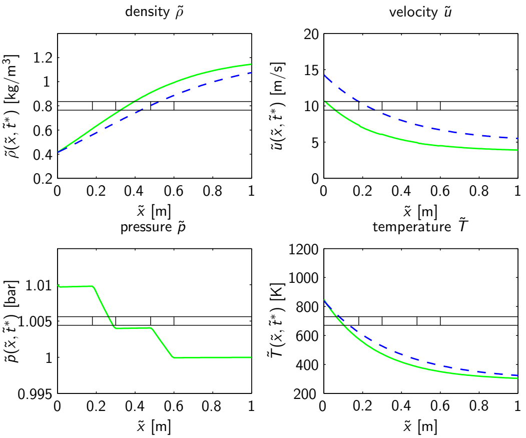


Figure: Example 1: Numerical results after $\tilde{t}^* = 0.4$s

Single pipe: Example 2

(FE) (AM)

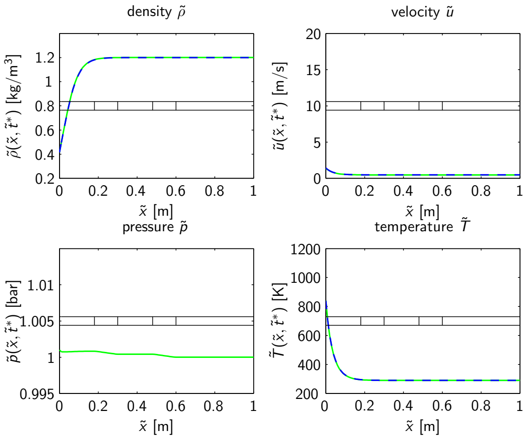


Figure: Example 2: Numerical results after $\tilde{t}^* = 3$s

Single pipe: Output data

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

	Example 1		Example 2	
	FE	AM	FE	AM
spatial supporting points	100	100	100	100
time steps	25947	617	**176644**	**488**
last time step size	1.5324e-05	0.00062999	1.6902e-05	0.0062657
computation time (in sec)	113.5494	0.29539	772.1798	0.24294
computation time (in min)	1.8925	0.0049232	12.8697	0.004049
largest speed (λ_{max}, $\tilde{u}_{max}$)	587.3086	4.2859	532.4936	1.4364
Mach number M	0.01828	0.02459	0.0022544	0.0024725
ratio FE/AM time steps	42.0535		361.9754	
ratio AM/FE time steps size	41.1111		370.7164	
ratio $\lambda_{max}/\tilde{u}_{max}$	41.1111		370.7164	
ratio FE/AM computation time	384.4039		**3178.4926**	

Table: Output data for example 1 and example 2. The computation time refers to a personal computer (Intel(R) Core(TM) i5 CPU 750 @ 2.67GHz) with 8 GB of memory

Motivation

Modeling

First model

Network approach

Network

Coupling conditions

Numerical simulation

Optimization

Conclusion

Whole exhaust pipe: Example 3

(FE) $c_N = 0.1$ (AM) $c_N = 0.1$ (AM) $c_N = 1$

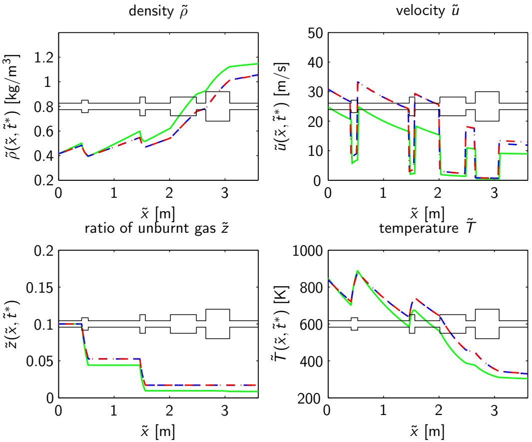


Figure: Example 3: Numerical results after $\tilde{t}^* = 2$s

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Whole exhaust pipe: Example 4

(FE) $c_N = 0.1$ (AM) $c_N = 0.1$ (AM) $c_N = 1$

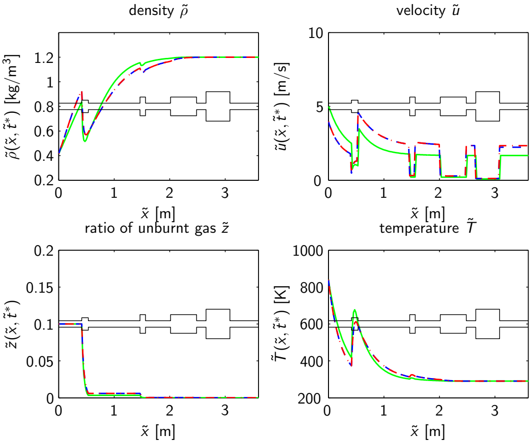


Figure: Example 4: Numerical results after $\tilde{t}^* = 3$s

Whole exhaust pipe: Output data

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

(FE) $c_N = 0.1$ (AM) $c_N = 0.1$ (AM) $c_N = 1$

	Example 3			Example 4		
	FE	AM		FE	AM	
spatial supp. points	200	200	(200)	200	200	(200)
time steps	392628	34052	(3469)	**570800**	6849	(**725**)
last time step size	4.98e-06	5.40e-05	(5.40e-04)	5.25e-06	3.91e-04	(3.91e-03)
comp. time (in sec)	5935.86	43.97	(4.75)	8587.31	9.96	(1.26)
comp. time (in min)	98.93	0.73	(0.08)	143.12	0.17	(0.02)
max speed ($\lambda_{max}, \tilde{u}_{max}$)	362.02	33.32	(33.28)	343.24	4.61	(4.61)
Mach number M	0.042	0.056	(0.056)	0.009	0.009	(0.009)
ratio FE/AM time steps	11.53 (113.18)			83.34 (787.31)		
ratio AM/FE Δt	10.83 (108.37)			74.34 (743.24)		
ratio $\lambda_{max}/\tilde{u}_{max}$	10.86 (10.88)			74.51 (74.53)		
ratio FE/AM comp. time	134.98 (1238.80)			861.58 (**6736.72**)		

Table: Output data for example 3 and example 4. The computation time refers to a personal computer (Intel(R) Core(TM) i5 CPU 750 @ 2.67GHz) with 8 GB of memory

Minor loss term: Example 5

$\theta = \pi$ $\theta = \pi/3$ no pressure loss

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Minor loss term: Example 5

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

$\theta = \pi$ $\theta = \pi/3$ no pressure loss

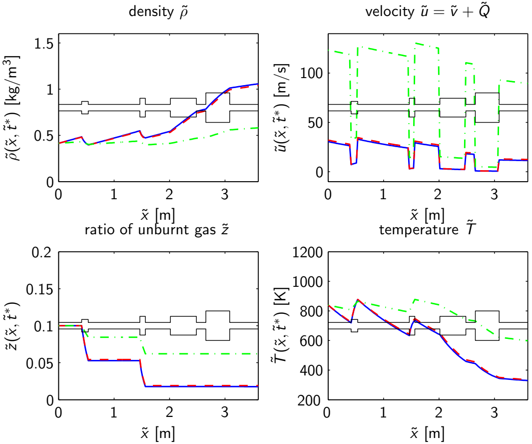


Figure: Example 5: Numerical results after $\tilde{t}^* = 2$s

Related Work

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

- accepted and to appear:

I. Gasser and M. Rybicki
Modelling and Simulation of Gas Dynamics in an Exhaust Pipe
Applied Mathematical Modelling, 2012.

- related work

I. Gasser and J. Struckmeier
An asymptotic-induced one-dimensional model to describe Fires in Tunnels
Mathematical methods in the applied sciences (25), p. 1231-1249, 2002.

I. Gasser and M. Kraft
Modelling and simulation of fires in tunnels
Networks in heterogeneous media (3), p. 691-707, 2008.

I. Gasser
Modelling and Simulation of a Solar Updraft Tower
Kinetic and Related Models (2), p. 191-204, 2009.

M. Bauer and I. Gasser
Modelling, Asymptotic Analysis, and Simulation of an Energy Tower
SIAM J. Appl. Math. (72), p. 362-381, 2012.

E. Felaco and I. Gasser
Modelling, Asymptotic Analysis and Simulation of the Gas Dynamics in a Chimney
submitted 2012

- planed

I. Gasser, M. Rybicki and W. Wollner
Optimal Control of Gas Temperature on Networks

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Optimization Problem

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

- **Aim:** "Heat up CC without using too much fuel“.

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Optimization Problem

- **Aim:** "Heat up CC without using too much fuel".
- **Equation for temperature in catalytic converter** required:

$$(T_c)_t = h_c(T_{\text{gas}} - T_c^i) \tag{8}$$

where T_{gas} is the mean gas temperature in the cc.

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Optimization Problem

- **Aim:** "Heat up CC without using too much fuel".
- **Equation for temperature in catalytic converter** required:

$$(T_c)_t = h_c(T_{gas} - T_c^i) \tag{8}$$

where T_{gas} is the mean gas temperature in the cc.

- Cost functional

$$\mathcal{J} := \frac{1}{2} \sum_{i \in C} \int_0^{t_{end}} (T_c^i(t) - T_{opt})^2 dt + \frac{\sigma}{2} \int_0^{t_{end}} z_l(t)^2 dt \tag{9}$$

Optimization Problem

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

- **Aim:** "Heat up CC without using too much fuel".
- **Equation for temperature in catalytic converter** required:

$$(T_c)_t = h_c(T_{gas} - T_c^i) \tag{8}$$

where T_{gas} is the mean gas temperature in the cc.

- Cost functional

$$\mathcal{J} := \frac{1}{2} \sum_{i \in C} \int_0^{t_{end}} (T_c^i(t) - T_{opt})^2 dt + \frac{\sigma}{2} \int_0^{t_{end}} z_l(t)^2 dt \tag{9}$$

- **Task:** Minimize Cost functional subject to the constraints.

Optimization Problem

- **Aim:** "Heat up CC without using too much fuel".
- **Equation for temperature in catalytic converter** required:

$$(T_c)_t = h_c(T_{\text{gas}} - T_c^i) \quad (8)$$

where T_{gas} is the mean gas temperature in the cc.

- Cost functional

$$\mathcal{J} := \frac{1}{2} \sum_{i \in C} \int_0^{t_{end}} (T_c^i(t) - T_{opt})^2 dt + \frac{\sigma}{2} \int_0^{t_{end}} z_l(t)^2 dt \quad (9)$$

- **Task:** Minimize Cost functional subject to the constraints.
- **Strategy:** First variations of Lagrange functional lead to an optimality system (KKT-condition)

Lagrangian functional

$$
\begin{aligned}
\mathcal{L} = & \frac{1}{2}\sum_{i\in C}\int_0^{t_{end}} (T_c^i(t) - T_{opt})^2 dt + \frac{\sigma}{2}\int_0^{t_{end}} z_l^1(t)^2 dt \\
& - \sum_{i=1}^{n_P}\int_0^{t_{end}}\int_0^{L^i} \xi_1^i(\rho_t^i + (v^i + Q^i)\rho_x^i + q^i\rho^i)dxdt - \sum_{i=1}^{n_P}\int_0^{t_{end}}\int_0^{L^i} \xi_2^i(z_t^i + (v^i + Q^i)z_x^i + z^i K(T^i))dxdt \\
& - \sum_{i=1}^{n_P}\int_0^{t_{end}} \xi_3^i \left(v_t^i - \frac{1}{R^i(0)}\left[p_{1\,l}^i - p_{1\,r}^i - \int_0^{L^i} \rho^i Q_t^i + \rho^i(v^i + Q^i)q^i + C_f \frac{\rho^i(v^i + Q^i)^2}{2} dx \right.\right. \\
& \qquad \left.\left. - C_c \int_0^{L^i} \rho^i(v^i + Q^i)\, dx \right]\right) dt - \sum_{i\in C}\int_0^{t_{end}} \xi_4^i((T_c^i)_t - h_c(T_{gas}^i - T_c^i))dt \\
& - \int_0^{t_{end}} \eta_1(\rho^1(0,t) - \rho_l(t))dt - \int_0^{t_{end}} \eta_2(z^1(0,t) - z_l(t))dt - \sum_{i=1}^{n_P}\int_0^{L^i} \nu_1^i(\rho^i(x,0) - \rho_{ic}^i(x))dx \\
& - \sum_{i=1}^{n_P}\int_0^{L^i} \nu_2^i(z^i(x,0) - z_{ic}^i(x))dx - \sum_{i=1}^{n_P} \nu_3^i(v^i(0) - v_{ic}^i) - \sum_{i=1}^{n_P} \nu_4^i(T_c^i(0) - T_{c\,ic}^i)
\end{aligned}
$$

Optimality system

- constraints or state equations

$$\begin{aligned} \rho_t^i + (v^i + Q^i)\rho_x^i &= -q^i \rho^i \\ z_t^i + (v^i + Q^i) z_x^i &= -z^i K(T^i) \\ v_t^i &= \Phi^i / R^i(0) \\ (T_c^i)_t &= h_c(T_{\text{gas}}^i - T_c^i) \end{aligned} \tag{10}$$

- adjoint or co-state equations

$$\begin{aligned} (\xi_1^i)_t + (v^i + Q^i)(\xi_1^i)_x &= \dots \\ (\xi_2^i)_t + (v^i + Q^i)(\xi_2^i)_x &= \dots \\ (\xi_3^i)_t &= \dots \\ (\xi_4^i)_t &= \dots \end{aligned} \tag{11}$$

- optimality condition

$$\sigma z_l + \eta_2 = 0 \tag{12}$$

Numerical approach

Algorithm

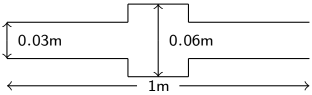
Guess a initial control $z_l^{(0)}$. *For* $k = 0, 1, 2, \dots$ *repeat the following steps until satisfactory convergence is achieved:*

1. *solve the constraints with control* $z_l^{(k)}$ *to obtain the corresponding state variables* $\rho^{(k)} = \rho(z_l^{(k)}), z^{(k)} = z(z_l^{(k)}), v^{(k)} = v(z_l^{(k)}), T_c^{(k)} = T_c(z_l^{(k)})$;
2. *solve the adjoint system with state variables* $\rho^{(k)}, z^{(k)}, v^{(k)}, T_c^{(k)}$ *to obtain the adjoint variables* $\xi_1^{(k)}, \xi_2^{(k)}, \xi_3^{(k)}, \xi_4^{(k)}, \eta_2^{(k)}$;
3. *use* $\eta_2^{(k)}$ *to compute gradient* $j'(z_l^{(k)})$;
4. *compute step length* α *via line search (*ARMIJO *or* WOLFE-POWELL *method);*
5. *set* $z_l^{(k+1)} = z_l^{(k)} - \alpha j'(z_l^{(k)})$.

2 numerical examples

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Setting:



$$T_{opt} = 600\text{K}$$
$$t_{end} = 60\text{s}$$

Examples:

1. low costs for boundary control variable, low starting value.

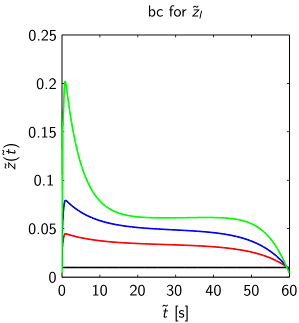
$$\sigma = 0.1 \qquad z_l^{(0)}(t) = 0.01 \ \ \forall t \in [0, t_{end}]$$

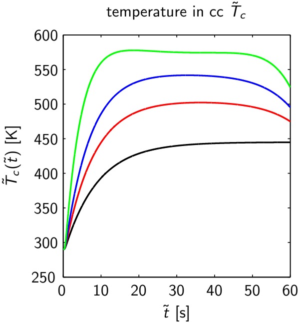
2. high costs for boundary control variable, high starting value.

$$\sigma = 1 \qquad z_l^{(0)}(t) = 0.1 \ \ \forall t \in [0, t_{end}]$$

Numerical simulations: Example 1

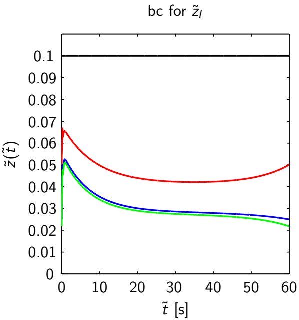
iteration	$\mathcal{J} = \sigma \mathcal{J}_z + \mathcal{J}_{T_c^2}$	$\mathcal{J}_z = \frac{1}{2} \int_0^{t_{end}} z_l(t)^2 dt$	$\mathcal{J}_{T_c^2} = \frac{1}{2} \int_0^{t_{end}} (T_c^2(t) - T_{opt})^2 dt$
0	118.873	3.000	118.574
1	69.106	31.863	65.920
2	47.542	73.588	40.183
9	35.306	171.433	18.162

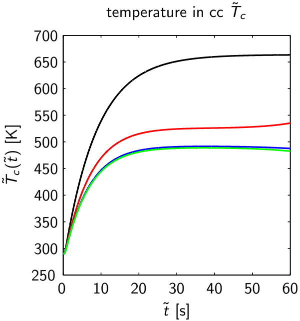




Numerical simulations: Example 2

iteration	$\mathcal{J} = \sigma \mathcal{J}_z + \mathcal{J}_{T_c^2}$	$\mathcal{J}_z = \frac{1}{2} \int_0^{t_{end}} z_l(t)^2 dt$	$\mathcal{J}_{T_c^2} = \frac{1}{2} \int_0^{t_{end}} (T_c^2(t) - T_{opt})^2 dt$
0	328.412	300.000	28.412
1	111.408	65.232	46.177
2	98.437	29.959	68.478
3	98.303	27.405	70.898





Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Conclusion

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

1. **Conclusion**
   - Inclusion of pressure loss terms possible with network approach
   - very good qualitative consistence of the asymptotic model with the full Euler model.
   - Much faster numerical simulations.
   - Optimization or control (e.g. of temperature) with respect to boundary conditions possible.

Conclusion

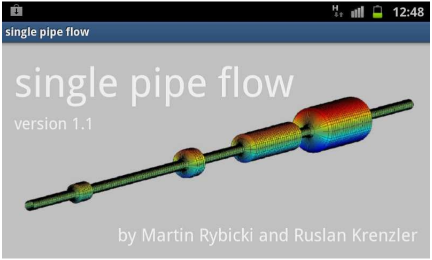
Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

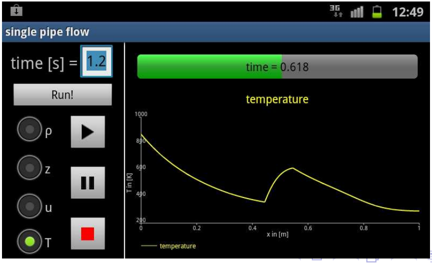
1. **Conclusion**
   - Inclusion of pressure loss terms possible with network approach
   - very good qualitative consistence of the asymptotic model with the full Euler model.
   - Much faster numerical simulations.
   - Optimization or control (e.g. of temperature) with respect to boundary conditions possible.
2. **Open Questions**
   - existence of a solution to the constraints
   - convergence of the optimization algorithm

Android App

Motivation
Modeling
First model
Network approach
Network
Coupling conditions
Numerical simulation
Optimization
Conclusion

Real-time simulations on a Smartphone





Motivation

Modeling
First model
Network approach

Network
Coupling conditions

Numerical simulation

Optimization

Conclusion