Development and Application of a Fast Quasi-Steady Solver for Integrated Modeling of Exhaust Aftertreatment Systems

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Modeling Solutions Overview

- Flow model to coupled reactor model
  *GUI based chemistry library*
  *(SAE 2007-01-4127, 9-10th Cleers Workshop)*

- Computational y efficient solver
  *Quasi-Steady (QS) solver*
  *(SAE 2008-01-0866)*

- Kinetic parameter calibration
  *DoE (Design of Experiment) or direct optimizer*
  *(SAE 2007-01-4127)*
• Advanced applications
  System modeling, effects of aging

• Fast models for SIL and HIL applications
  From detailed model to NN model
  (SIA, 28-29th May, 2008, INSA de Rouen, France)

• Multi-dimensional and quasi-dimensional solution
  QS based 2D/3D modeling
### Flow Model to Reactor Model

#### Reactants and Products

<table>
<thead>
<tr>
<th>Reactants</th>
<th>Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO + 0.5CO2</td>
<td>CO2</td>
</tr>
<tr>
<td>C3H8 + 4.5CO2</td>
<td>3CO2 + 3H2O</td>
</tr>
</tbody>
</table>

#### Pre-exponent Multiplier

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Pre-exponent Multiplier</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaCO3 + 2NO2 + 5CO2</td>
<td>1500</td>
</tr>
<tr>
<td>BaCO3 + 2NO + 1.5CO2</td>
<td>17000</td>
</tr>
<tr>
<td>Ba(NO3)2 + 3CO2</td>
<td>2.0E14</td>
</tr>
<tr>
<td>Ba(NO3)2 + H2 + 2CO2</td>
<td>0</td>
</tr>
<tr>
<td>NO + 0.5CO2</td>
<td>9.0E9</td>
</tr>
<tr>
<td>NO2 + NO + 0.5CO2</td>
<td>5.0E10</td>
</tr>
<tr>
<td>CO + NO</td>
<td>9.0E17</td>
</tr>
</tbody>
</table>

#### Temperature Exponent

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Temperature Exponent</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaCO3 + 2NO2 + 5CO2</td>
<td>0</td>
</tr>
<tr>
<td>BaCO3 + 2NO + 1.5CO2</td>
<td>0</td>
</tr>
<tr>
<td>Ba(NO3)2 + 3CO2</td>
<td>0</td>
</tr>
<tr>
<td>Ba(NO3)2 + H2 + 2CO2</td>
<td>0</td>
</tr>
<tr>
<td>NO + 0.5CO2</td>
<td>-1</td>
</tr>
<tr>
<td>NO2 + NO + 0.5CO2</td>
<td>-1</td>
</tr>
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</table>

#### Activation Temperature

<table>
<thead>
<tr>
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<th>Activation Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaCO3 + 2NO2 + 5CO2</td>
<td>600</td>
</tr>
<tr>
<td>BaCO3 + 2NO + 1.5CO2</td>
<td>500</td>
</tr>
<tr>
<td>Ba(NO3)2 + 3CO2</td>
<td>400</td>
</tr>
<tr>
<td>Ba(NO3)2 + H2 + 2CO2</td>
<td>400</td>
</tr>
<tr>
<td>NO + 0.5CO2</td>
<td>8412.25</td>
</tr>
<tr>
<td>NO2 + NO + 0.5CO2</td>
<td>8412.25</td>
</tr>
</tbody>
</table>

#### Concentration Expressions

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Concentration Expressions</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaCO3 + 2NO2 + 5CO2</td>
<td>(NO2)2*(O2)^0.5</td>
</tr>
<tr>
<td>BaCO3 + 2NO + 1.5CO2</td>
<td>(NO)^0.5*(O2)^1.5</td>
</tr>
<tr>
<td>Ba(NO3)2 + 3CO2</td>
<td>{CO}^3.0</td>
</tr>
<tr>
<td>Ba(NO3)2 + H2 + 2CO2</td>
<td>{CO2}*(H2)^0.5</td>
</tr>
<tr>
<td>NO + 0.5CO2</td>
<td>{NO}</td>
</tr>
<tr>
<td>NO2 + NO + 0.5CO2</td>
<td>{NO2}</td>
</tr>
</tbody>
</table>

#### Coverage Expression

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Coverage Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaCO3 + 2NO2 + 5CO2</td>
<td>4(1)</td>
</tr>
<tr>
<td>BaCO3 + 2NO + 1.5CO2</td>
<td>4(1)</td>
</tr>
<tr>
<td>Ba(NO3)2 + 3CO2</td>
<td>1-4(1)</td>
</tr>
<tr>
<td>Ba(NO3)2 + H2 + 2CO2</td>
<td>1-4(1)</td>
</tr>
<tr>
<td>NO + 0.5CO2</td>
<td>1</td>
</tr>
<tr>
<td>NO2 + NO + 0.5CO2</td>
<td>1</td>
</tr>
</tbody>
</table>

#### Concentration Expressions

<table>
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</tr>
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<td>(NO2)2*(O2)^0.5</td>
</tr>
<tr>
<td>BaCO3 + 2NO + 1.5CO2</td>
<td>(NO)^0.5*(O2)^1.5</td>
</tr>
<tr>
<td>Ba(NO3)2 + 3CO2</td>
<td>{CO}^3.0</td>
</tr>
<tr>
<td>Ba(NO3)2 + H2 + 2CO2</td>
<td>{CO2}*(H2)^0.5</td>
</tr>
<tr>
<td>NO + 0.5CO2</td>
<td>{NO}</td>
</tr>
<tr>
<td>NO2 + NO + 0.5CO2</td>
<td>{NO2}</td>
</tr>
</tbody>
</table>

#### Langmuir-Hinshelwood Expressions

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Langmuir-Hinshelwood Expressions</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO + 0.5O2</td>
<td>1.0 + 65.6<em>exp(651.0/T)^0.5</em>{CO} + 1.0<em>exp(651.0/T)^0.5</em>{C3H8}</td>
</tr>
<tr>
<td>CO + 0.5O2</td>
<td>1.0 + 3.95<em>exp(1161.0/T)^0.5</em>{CO} + 2.0*{C3H8}^2.0</td>
</tr>
<tr>
<td>CO + 0.5O2</td>
<td>1.0 + 4.79<em>exp(3733.0/T)^0.7</em>{NO} + 0.7</td>
</tr>
<tr>
<td>CO + 0.5O2</td>
<td>1.0 + 19.96<em>exp(654.5/T)^0.5</em>{CO}</td>
</tr>
<tr>
<td>CO + 0.5O2</td>
<td>1.0 + 65.6<em>exp(651.0/T)^0.5</em>{CO} + 1.0<em>exp(651.0/T)^0.5</em>{H2}</td>
</tr>
</tbody>
</table>
Simulation Workflow

Experiment => calibration => Prediction

Start

GT-POWER model

GT-POWER solver

Online sensors/controls evaluating objective

Altered parameters

Yes/no

Built-in DoE or Direct Optimizer

End

Initial parameters

Values

objective function

Applied to TWC

Light-off Data

before

after

cycle emissions prediction

All in a one integrated environment
Computational Efficiency of Q-S Solver (SAE 2008-01-0866)

- TWC kinetic model
- Simulation duration: 2942 seconds
- 20 sub-volume, dt = 0.1 seconds
- QS can be 10-100 times faster than real time

\[ 0 = \frac{\partial F(U)}{\partial z} + G(U) \]
\[ \frac{\partial U(z,t)}{\partial t} = \frac{\partial F(U)}{\partial z} + G(U) \]

RT threshold

Quasi-Steady    Operator-Splitting
Accuracy of QS Approach

\[ \frac{\partial C_g}{\partial t} + u \frac{\partial C_g}{\partial z} = \dot{R}(C_s, \theta, T_s) \]

\[ u \frac{\partial C_g}{\partial z} = \dot{R}(C_s, \theta, T_s) - \frac{C_g - C_g^0}{\Delta t} = \dot{R}'(C_s, \theta, T_s) \]
Component Level Modeling
Zeolite Based SCR

- Experimental data was provided by PSA Peugeot Citroën
- Five set of calibration data aimed at determination of parameters involving
  - Test 1: Storage capacity, absorption/desorption
    \[ \cdot \ + \ \text{NH}_3 \ \leq \ \Rightarrow \ \cdot \text{NH}_3 \]
  - Test 2: Ammonia oxidation
    \[ 4\text{NH}_3 + 3\text{O}_2 \Rightarrow 2\text{N}_2 + 6\text{H}_2\text{O} \]
  - Test 3: “Standard” SCR reaction
    \[ 4\text{NH}_3 + 4\text{NO} + \text{O}_2 \Rightarrow 4\text{N}_2 + 6\text{H}_2\text{O} \]
  - Test 4: “Slow” SCR reaction
    \[ 8\text{NH}_3 + 6\text{NO}_2 = \Rightarrow 7\text{N}_2 + 12\text{H}_2\text{O} \]
  - Test 5: “Fast” SCR reaction
    \[ 4\text{NH}_3 + 2\text{NO} + 2\text{NO}_2 \Rightarrow 4\text{N}_2 + 6\text{H}_2\text{O} \]
SGB protocol for testing SCR catalyst

- Purge under N2
- Start NH3 Injection
- Stop NH3 and Begin NOx introduction

Concentrations vs. Time (s) and Temperature
Processed NH3 and Pollutant Sensors Data

Test 1: Absorption/Desorption without O2
- NH3 inlet
- NH3 outlet

Test 2: Absorption/Desorption with O2
- NH3 inlet
- NH3 outlet

Test 3: "Standard"
- NH3 inlet
- NH3 outlet
- NOx inlet
- NOx outlet

Test 4: "Slow"
- NH3 inlet
- NH3 outlet
- NOx inlet
- NOx outlet

Test 5: "Fast"
- NH3 inlet
- NH3 outlet
- NOx inlet
- NOx outlet
Calculation of Storage Capacity

Inlet NH₃

Outlet NH₃

Test 4: adsorption of NH₃ without O₂
Storage Capacity (cont.)

- Experimental results suggest more NH$_3$ desorbed than could be accounted for by storage
- Two possibilities exist:
  1. experimental error in one or both NH$_3$ sensors
  2. NH$_3$ is pre-stored
Storage Capacity (cont.)

• The onset of saturation and shape of saturation curve indicated by the exit NH₃ sensor seemed to be consistent

• Optimization was performed to determine:
  – storage capacity
  – pre-stored NH₃ (if any)

• Optimization goal:
  – conserve NH₃ mass
  – conserve onset/shape of NH₃ saturation curve

• Built-in direct optimizer (Brent) was used
Storage Capacity (cont.)

- A pre-storage corresponding to 45% coverage and a storage capacity of 4.9E-3gmole/m^2 were determined.
- These generally agree with all experiments.
Standard Reaction

$$4\text{NH}_3 + 4\text{NO} + \text{O}_2 \Rightarrow 4\text{N}_2 + 6\text{H}_2\text{O}$$
Fast Reaction

\[ 4\text{NH}_3 + 2\text{NO} + 2\text{NO}_2 \Rightarrow 4\text{N}_2 + 6\text{H}_2\text{O} \]
SCR NO\textsubscript{x} Selectivity Study

- NO\textsubscript{x} conversion should be highest at NO\textsubscript{2}/NO\textsubscript{x} ratio of 0.5 (or NO:NO\textsubscript{2} = 1:1)
- Study was performed using
  - Vary NO\textsubscript{2}/NO\textsubscript{x} ratio from 0-1
  - Vary temperature from 400-700K
  - 10 ppm NH\textsubscript{3} slip
  - 150 ppm NO\textsubscript{x}, NH\textsubscript{3} (variable), 10% H\textsubscript{2}O, 10% O\textsubscript{2}, balance N\textsubscript{2}
  - Constant volume flow rate = 0.55 liter/s
SCR NO\textsubscript{x} Selectivity Study

![Graph showing NOx Conversion vs NO2/NOx Ratio](image)

- **Solution Overview**
- **Calibration**
- **Q-S Solver**
- **SCR DOC**
- **Aged DOC**
- **SIL/HIL /NN**
- **2D/3D Model**
- **Conclusions**
Transient Emission Predictions

• Calibrated SCR model used for Transient NDEC cycle
• Model ran under two conditions:
  – Absorption site 100% “open” (no NH₃ prestorage)
  – Absorption site 0.0% “open”
Emission Predictions (cont.)

- All sites “open” (no NH$_3$ prestored)

- Cumulative Mass Changes:
  \[ \text{NO} = -28\% \quad \text{NO}_x = -37\% \]
  \[ \text{NO}_2 = -49\% \quad \text{NH}_3 = -100\% \]
**Computational Efficiency: SCR**

- Simulations were performed on a Pentium 4 3.4GHz processor with 1 GB of RAM

<table>
<thead>
<tr>
<th></th>
<th>Time Step Size (s)</th>
<th>Simulation Time (s)</th>
<th>Computational Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abs/Des without O2</td>
<td>0.50</td>
<td>3654</td>
<td>31</td>
</tr>
<tr>
<td>Abs/Des with O2</td>
<td>0.50</td>
<td>3654</td>
<td>43</td>
</tr>
<tr>
<td>Standard Reaction</td>
<td>0.50</td>
<td>3654</td>
<td>45</td>
</tr>
<tr>
<td>Slow Reaction</td>
<td>0.50</td>
<td>3654</td>
<td>49</td>
</tr>
<tr>
<td>Fast Reaction</td>
<td>0.50</td>
<td>3654</td>
<td>57</td>
</tr>
<tr>
<td>Transient without NH$_3$ prestored</td>
<td>0.25</td>
<td>1166</td>
<td>85</td>
</tr>
<tr>
<td>Transient with NH$_3$ prestored</td>
<td>0.25</td>
<td>1166</td>
<td>87</td>
</tr>
</tbody>
</table>

Simulations were performed on a Pentium 4 3.4GHz processor with 1 GB of RAM.
Component Level Modeling: DOC

- Step 1: Kinetic model calibration

Experiment was done at PSA Peugeot Citroen
NEDC Test Cycle Emissions: DOC

- Step 2: Emission predictions
  - Transient NEDC cycle
    - Cumulative mass conversions predicted to be:
      - CO = 61%
      - HC = 49%
      - NO = 6%
Computational Efficiency: DOC

- Simulations were performed on a Pentium 4 3.4GHz processor with 1 GB of RAM

<table>
<thead>
<tr>
<th>Step</th>
<th>Time Step Size (s)</th>
<th>Simulation Time (s)</th>
<th>Computational Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step 1: Calibration</td>
<td>0.25</td>
<td>327</td>
<td>11</td>
</tr>
<tr>
<td>Step 2: Prediction</td>
<td>0.25</td>
<td>1200</td>
<td>71</td>
</tr>
</tbody>
</table>

Simulations were performed on a Pentium 4 3.4GHz processor with 1 GB of RAM.
Aged DOC Modeling

Gas Exp 1

<table>
<thead>
<tr>
<th>Gas</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO (ppm)</td>
<td>1000</td>
</tr>
<tr>
<td>C\textsubscript{2}H\textsubscript{4} (ppm)</td>
<td>300</td>
</tr>
<tr>
<td>H\textsubscript{2} (ppm)</td>
<td>333</td>
</tr>
<tr>
<td>NO\textsubscript{2} (ppm)</td>
<td>100</td>
</tr>
<tr>
<td>NO (ppm)</td>
<td>0</td>
</tr>
<tr>
<td>H\textsubscript{2}O (Vol.-%)</td>
<td>4.5</td>
</tr>
<tr>
<td>CO\textsubscript{2} (Vol.-%)</td>
<td>5</td>
</tr>
<tr>
<td>O\textsubscript{2} (Vol.-%)</td>
<td>10</td>
</tr>
</tbody>
</table>

*Balance consists of N\textsubscript{2}*

Measurements from Santhoji and coworkers:

"Aged DOC is a Net Consumer of NO\textsubscript{2}: Analysis of Vehicle, Engine-dynamometer and Reactor Data", SAE NO. 2007-01-3984
Aged DOC Modeling

Measurements from Santhoji and coworkers:
"Aged DOC is a Net Consumer of NO2: Analysis of Vehicle, Engine-dynamometer and Reactor Data", SAE NO. 2007-01-3984
Aged DOC Modeling

• Introduce additional reactions:

**R1:** \( CO + NO_2 \rightarrow CO_2 + NO \)

**R2:** \( C_2H_4 + 4NO_2 \rightarrow 2CO_2 + 6NO + 2H_2O \)

**R3:** \( C_2H_4 + 6NO_2 \rightarrow 2CO_2 + 3N_2 + 2H_2O \)
Aged DOC Modeling

R1: CO + NO₂ ⇒ CO₂ + NO

Exp. ..............

Sim.  ___________

R2: C₂H₄ + 4NO₂ ⇒ 2CO₂ + 6NO + 2H₂O

R3: C₂H₄ + 6NO₂ ⇒ 2CO₂ + 3N₂ + 2H₂O

Measurements from Santhoji and coworkers:
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Aged DOC Modeling

Exp. .......... Sim.

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Aged DOC Modeling

Experimental inlet conditions provided by PSA Peugeot Citroen

Model predicts cumulative NO₂ reduction = 44%
Neural Network Training

- Three-Layer Feedforward Neural Network
  - 2 hidden layers with tan-sigmoid activation functions
  - 1 output layer with linear activation function
- Levenberg-Marquardt algorithm for training
- Excellent Neural Network generalization capability
  - Fixed balanced penalties
  - Adjustable penalties ("Bayesian Regularization")
Conversion Efficiency

- DOC

### Graphs

- **CO conversion ratio**
- **HC conversion ratio**
- **NO concentration**
- **NO2 concentration**
Conversion Efficiency

• SCR

- NO conversion ratio
- NO2 conversion ratio
- NH3 slippage ratio
SIL/HIL Enabled Engine/NN-AT Model
### Computational Speed Comparison (1180s NDEC)

<table>
<thead>
<tr>
<th>Model Type</th>
<th>Solver</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standalone Kinetic AT</td>
<td>QS</td>
<td>90s</td>
</tr>
<tr>
<td>Standalone Neural Network AT</td>
<td>Explicit</td>
<td>2s</td>
</tr>
<tr>
<td>Detailed Engine + Kinetic AT</td>
<td>Explicit</td>
<td>60h</td>
</tr>
<tr>
<td>MV Engine + Kinetic AT</td>
<td>Explicit</td>
<td>39h</td>
</tr>
<tr>
<td>MV Engine (Explicit) + Kinetic AT (QS)</td>
<td>Mixed</td>
<td>635s</td>
</tr>
<tr>
<td>MV Engine + Neural Network AT</td>
<td>Explicit</td>
<td>625s</td>
</tr>
<tr>
<td>MV Engine + Neural Network AT</td>
<td>GT-Suite RT</td>
<td>331s</td>
</tr>
</tbody>
</table>
Pseudo-Multi-D Methodologies

Are real time 3-D simulations possible?

3D - vs- 1D

– Based on thermal object
  • Explicit discretization
  • Discretized CatalystBrick and thermal objects

– Based on Mathematical formulation (3-D conduction solution)
  • Implicit discretization
  • Diesel particulate filters
Aftertreatment Simulation

- **Modeling Techniques**
  - 3D: model discretized in X, Y, and Z direction
    - captures heat loss to environment
    - allows for non-uniform inlet flow
    - most computationally demanding

Inlet Flow
Aftertreatment Simulation
Representative Channel Approach

Solution Overview

Calibration

Q-S Solver

SCR

DOC

Aged DOC

SIL/HIL/NN

2D/3D Model

Conclusions
Typical Transient 2D Results

Warm-up

Regeneration
Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)  

Non-uniform Flow Distributions

Physical layout out

Pseudo front inlet mass flow rate intensity

(A)  

(B)
Typical Transient 3D Results

Non-uniform front inlet mass flow rate intensity

Loading Density at 110 sec. (g/L)
Typical Transient 2D Results
DPF Regeneration Animation
**Conclusion**

- A *Quasi-steady* (QS) based solver have been implemented that conserves accuracy of the computationally demanding fully explicit solver.

- Calibration of global kinetics was shown to be computationally efficient using DOE direct optimizers.

- Feasibility of SIL/HIL compatible model generation was demonstrated using detailed kinetic model.

- Various levels of modeling were demonstrated: *Detailed engine/vehicle* + detailed kinetics to *mean-value engine/vehicle* + NN/AT model.

- 1-D methodology was extended to simulate multi-dimensional effects using QS based quasi 2D/3D development.
1-D Catalyst Simulation
2-D Catalyst Simulation
Solution Overview
Calibration
Q-S Solver
SCR
DOC
Aged DOC
SIL/HIL /NN
2D/3D Model
Conclusions

Computational Speed Consideration

With regeneration rxn
Axial nodes = 21
300 second duration
dt = 0.1 sec.
AMD 1.8 GHz, 1.28 GB RAM

Real time is POSSIBLE for 2D/3D AT simulation