Simulating advantages of a LNT + passive SCR system with a bypass concept

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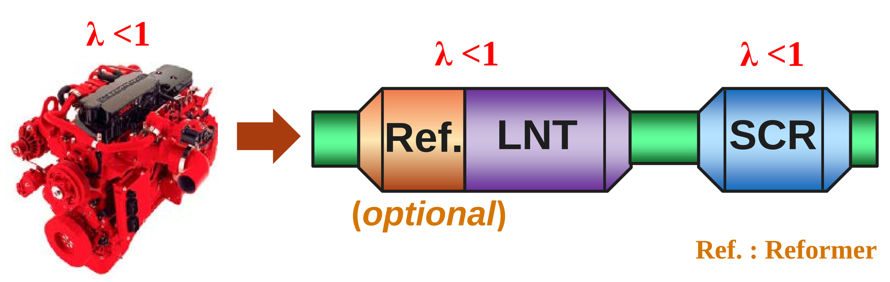
Motivation

❖ Conventional single-path concept for LNT + passive SCR systems

- High fuel penalty
- Limited NH_3 yield
- Reductants (CO/HC/H_2) slippage
- Catalyst durability concerns
- Complex engine control

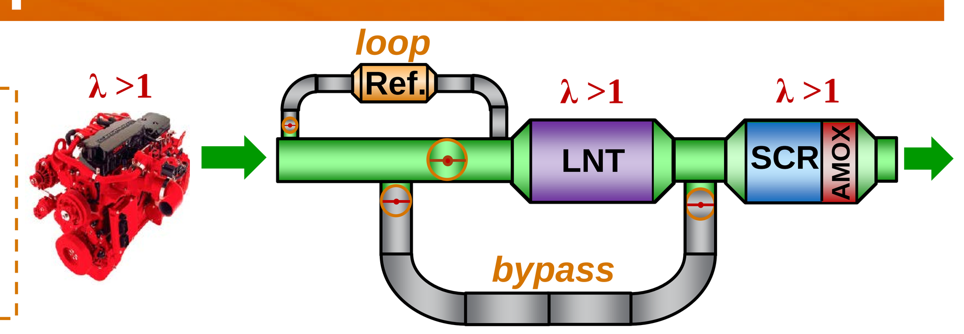


Challenging to meet upcoming both fuel economy and emission standards!

Bypass concept with a fuel reformer

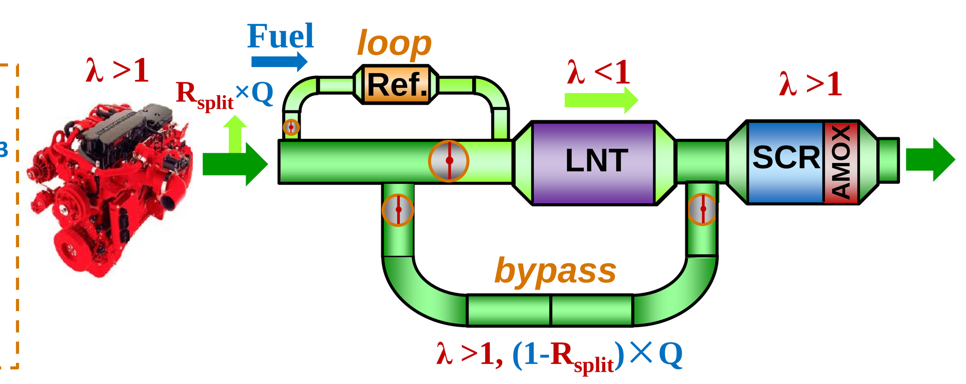
Lean mode

Engine:	λ > 1	AMOX:	λ > 1
LNT:	λ > 1	Reformer:	inactive
	NOx-Adsorption	Bypass:	closed
SCR:	λ > 1	Loop:	closed
	NOx-Reduction		



Rich mode

Engine:	λ > 1	AMOX:	λ > 1
LNT:	λ < 1		CO/H_2/HC/NH_3
	NOx-Desorption		Oxidation
	NH_3-Generation	Reformer:	active
SCR:	λ > 1	Bypass:	open
	NH_3-Adsorption	Loop:	open
	NOx-Reduction		



Potential benefits:

- Engine-independent LNT regeneration
- Low fuel consumption with high NH_3 yield
- Constant lean downstream LNT
- Better catalyst durability

Model equations

Fluid phase balance

$$\frac{\partial X_{fm,j}}{\partial t} = -u\frac{\partial X_{fm,j}}{\partial x} - \frac{k_{mo,j}}{R_\Omega}\left(X_{fm,j} - \langle X_{s,j}\rangle\right); \quad \rho_f Cpf\frac{\partial T_f}{\partial t} = -u\rho_f Cpf\frac{\partial T_f}{\partial x} - \frac{h}{R_\Omega}(T_f - T_s)$$

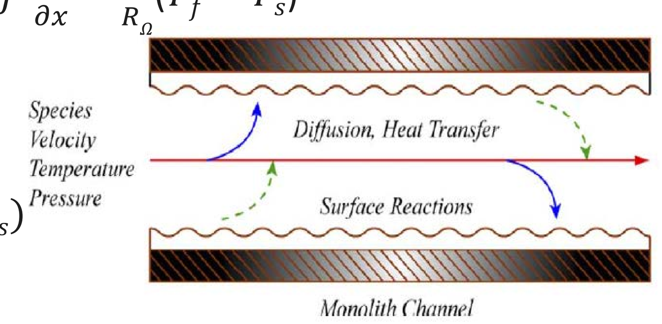
Washcoat phase balance

$$\epsilon_w\frac{\partial\langle X_{s,j}\rangle}{\partial t} = \frac{1}{C_{Total}}\sum_{r=1}^{rxn}\vartheta_{jr}R_r(\langle X_s\rangle,\theta,T_s) + \frac{k_{mo,j}}{\delta_c}\left(X_{fm,j} - \langle X_{s,j}\rangle\right);$$

$$\rho_w Cpw\frac{\partial T_s}{\partial t} = -k_w\frac{\partial^2 T_s}{\partial x^2} + \frac{h}{\delta_w}(T_f - T_s) + \frac{\delta_c}{\delta_w}\sum_{r=1}^{rxn}(-\Delta H)R_r(\langle X_s\rangle,\theta,T_s)$$

Site balance

$$C_S\frac{\partial\theta_i}{\partial t} = \sum_{r=1}^{rxn}\vartheta_{ir}R_r(\langle X_s\rangle,\theta,T_s)$$



Reaction scheme

LNT model

NOx storage
1) $NO + O_2 \leftrightarrow NO_2$
2) $BaCO_3 + 2NO_2 + 0.5\,O_2 \rightarrow Ba(NO_3)_2 + CO_2$

Stored NOx release
3) $Ba(NO_3)_2 + 3CO \rightarrow BaCO_3 + 2NO + 2CO_2$
4) $Ba(NO_3)_2 + 3H_2 + CO_2 \rightarrow BaCO_3 + 2NO + 3H_2O$
5) $Ba(NO_3)_2 + 1/3C_3H_6 \rightarrow BaCO_3 + 2NO + H_2O$
6) $Ba(NO_3)_2 + 3CO \rightarrow BaCO_3 + 2NO_2$
7) $Ba(NO_3)_2 + H_2 + CO_2 \rightarrow BaCO_3 + 2NO_2 + H_2O$

Reductant oxidation
8) $CO + 0.5O_2 \rightarrow CO_2$
9) $H_2 + 0.5O_2 \rightarrow H_2O$
10) $C_3H_6 + 4.5O_2 \rightarrow 3CO_2 + 3H_2O$

NOx reduction
11) $CO + NO \rightarrow 0.5N_2 + CO_2$
12) $H_2 + NO \rightarrow H_2O + 0.5N_2$
13) $C_3H_6 + 9NO \rightarrow 3H_2O + 4.5N_2 + 3CO_2$

N_2O formation
14) $CO + 2NO \rightarrow N_2O + CO_2$

NH_3 formation and consumption
15) $NO + 2.5H_2 \rightarrow NH_3 + H_2O$
16) $10/3NH_3 + Ba(NO_3)_2 + CO_2 \rightarrow BaCO_3 + 5H_2O + 8/3N_2$

SCR model

NH_3 adsorption and desorption
1) $NH_3 + S \rightarrow NH_3\text{-}S$
2) $NH_3\text{-}S \rightarrow NH_3 + S$

NH_3 oxidation
3) $NH_3\text{-}S + 0.75O_2 \rightarrow 0.5N_2 + 1.5H_2O + S$

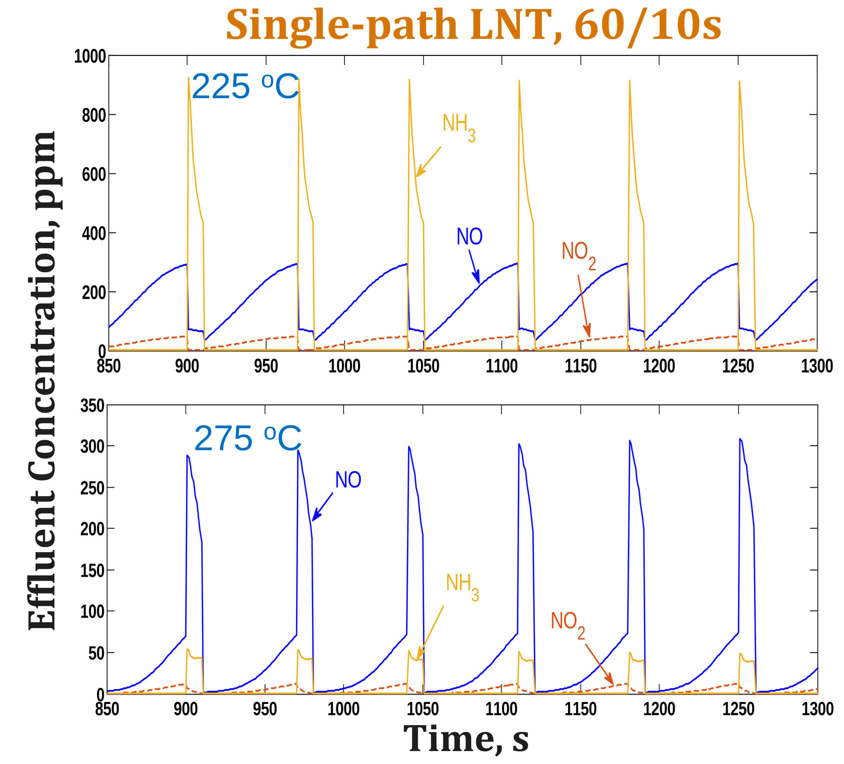
NO oxidation
4) $NO + 0.5O_2 \leftrightarrow NO_2$

SCR reactions
5) $4NH_3\text{-}S + 4NO + O_2 \rightarrow 4N_2 + 4S + 6H_2O$
6) $2NH_3\text{-}S + NO + NO_2 \rightarrow 2N_2 + 2S + 3H_2O$
7) $4NH_3\text{-}S + 3NO_2 \rightarrow 3.5N_2 + 4S + 6H_2O$

N_2O formation
8) $2NH_3\text{-}S + 2NO_2 \rightarrow N_2 + 2S + NH_4NO_3 + H_2O$
9) $NH_4NO_3 \rightarrow N_2O + 2H_2O$

Model validation

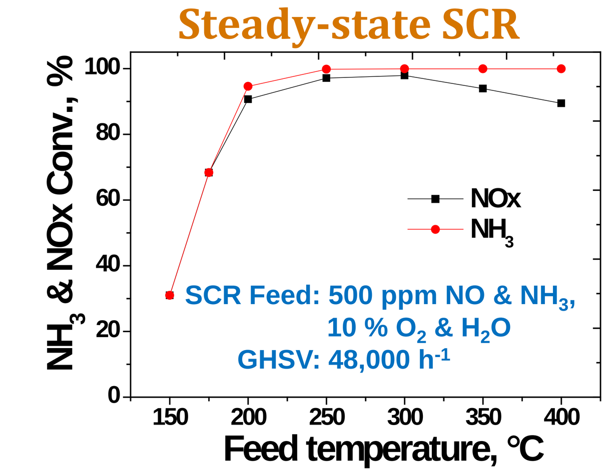
Single-path LNT, 60/10s



Feed condition

Gas	Lean	Rich
NO	500 ppm	500 ppm
O_2	10%	1%
H_2	–	1.2%
CO	–	1.2%
C_3H_6	–	500 ppm
GHSV	60,000h^{-1}	

Steady-state SCR

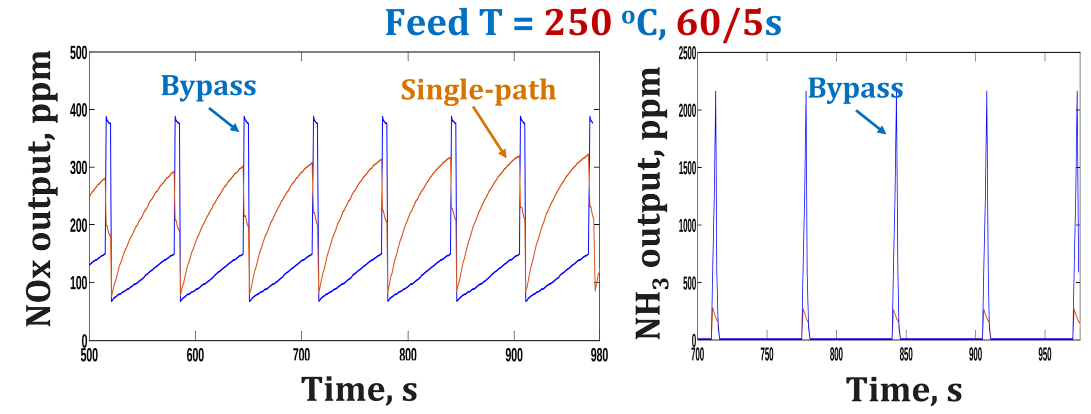


- Individually calibrated LNT and SCR models able to predict the typical experimental trends, respectively.

LNT regeneration: bypass vs. single-path

❖ Bypass concept for local LNT enrichment

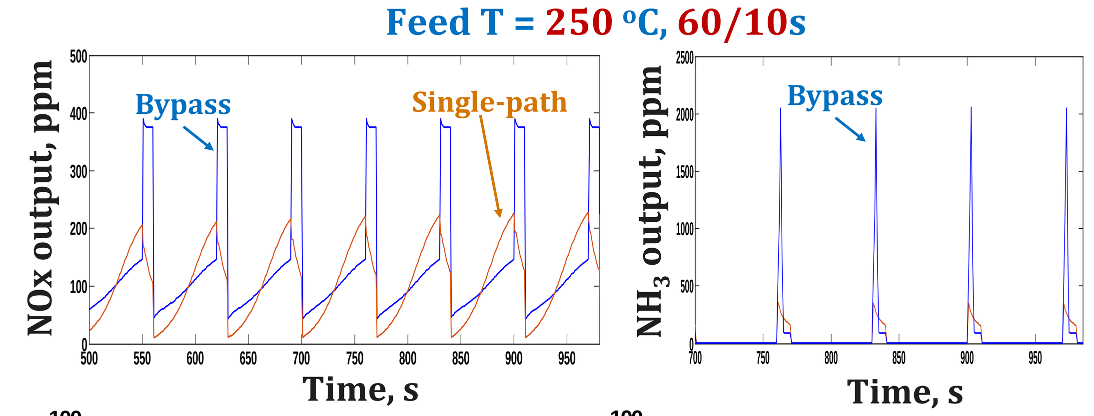
Feed T = 250 °C, 60/5s

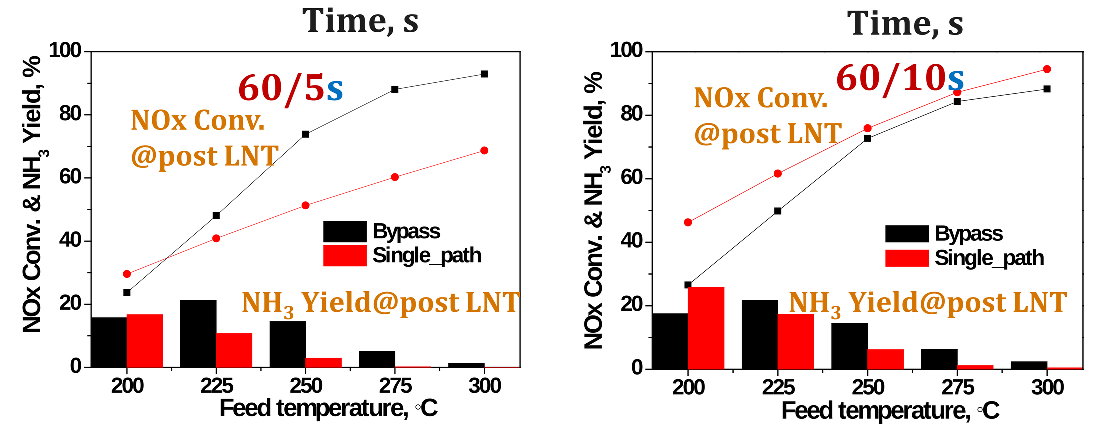


R_{split} = 1/4, fixed total reductant

Gas	Lean	Rich (LNT)
NO	500 ppm	500 ppm
O_2	10%	1%
H_2	–	4×1.2%
CO	–	4×1.2%
C_3H_6	–	4×500 ppm
GHSV	60,000h^{-1}	15,000h^{-1}

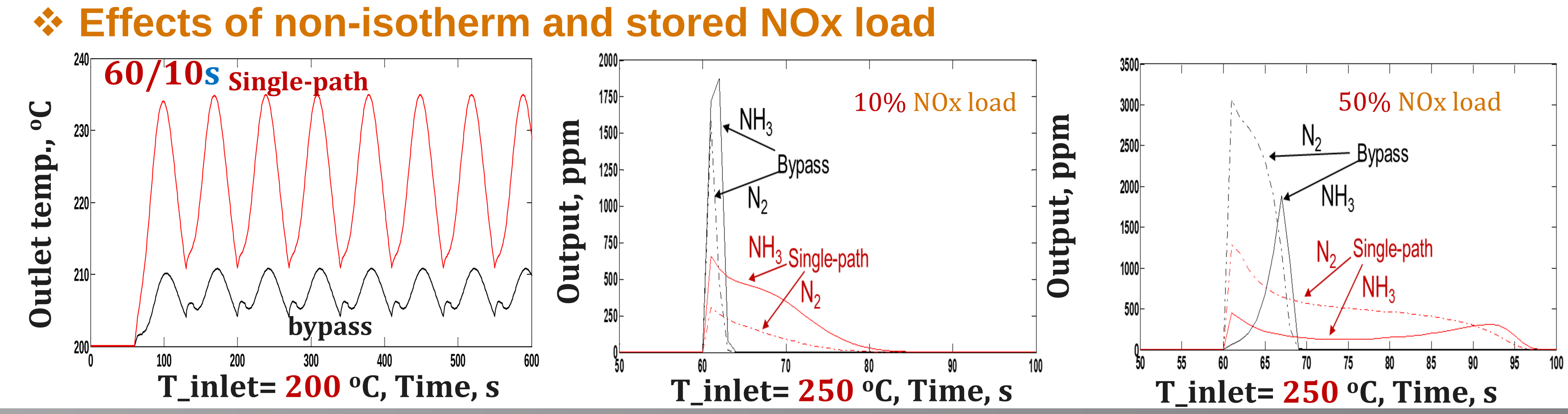
Feed T = 250 °C, 60/10s





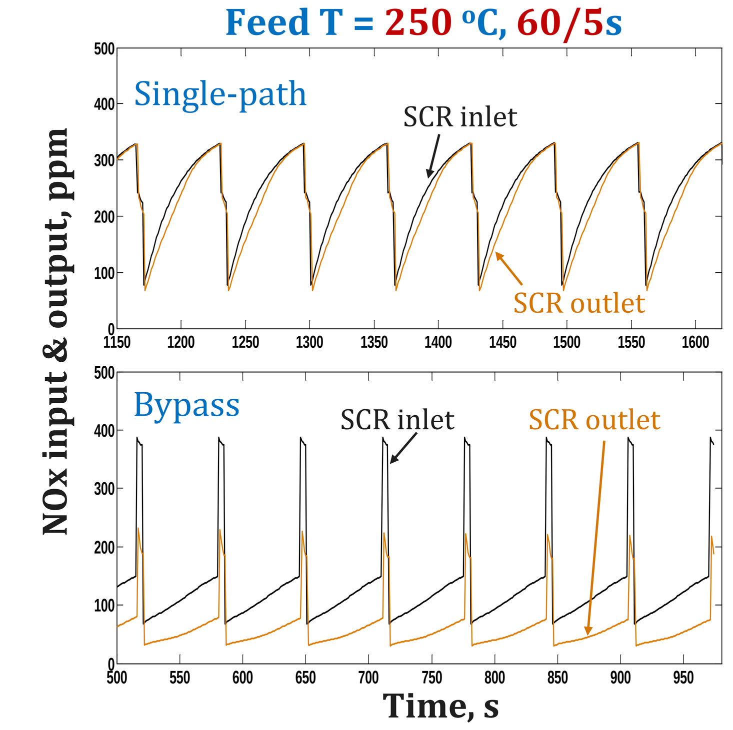
- Bypass concept enables higher NH_3 yield and NOx conversion for 60/5s cycling timing with a lower fuel penalty
- In contrast to single path, prolonged rich duration does not benefit bypass concept in terms of lower NOx conversion.
- Bypass concept enables rapid regeneration with higher NH_3 selectivity at low NOx load.

❖ Effects of non-isotherm and stored NOx load

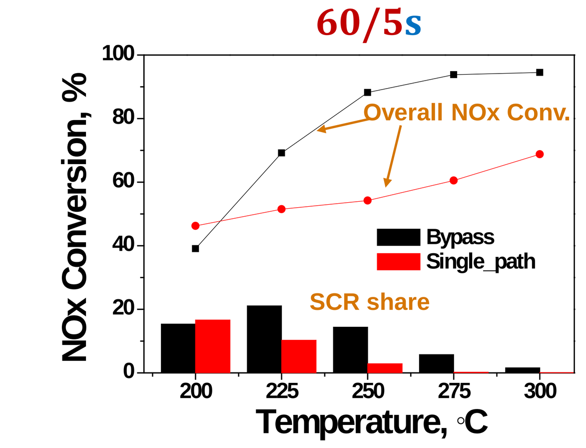


Combined LNT + SCR

Feed T = 250 °C, 60/5s



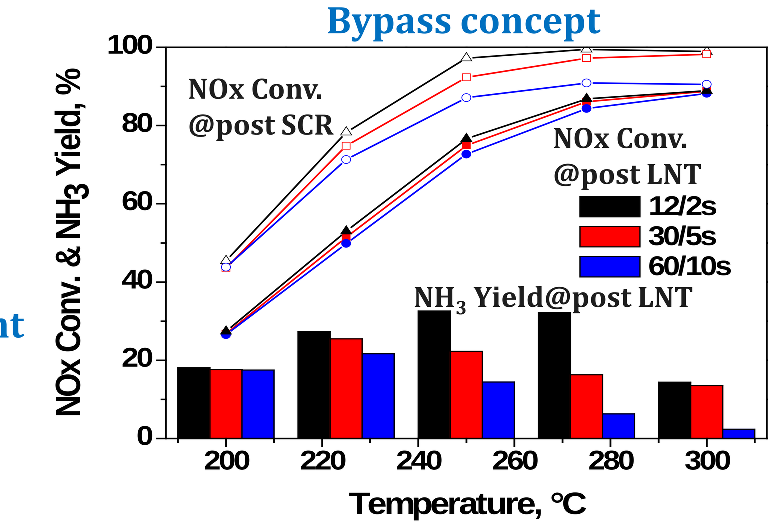
60/5s



- Bypass concept delivers higher overall NOx conversions with a higher SCR contribution.

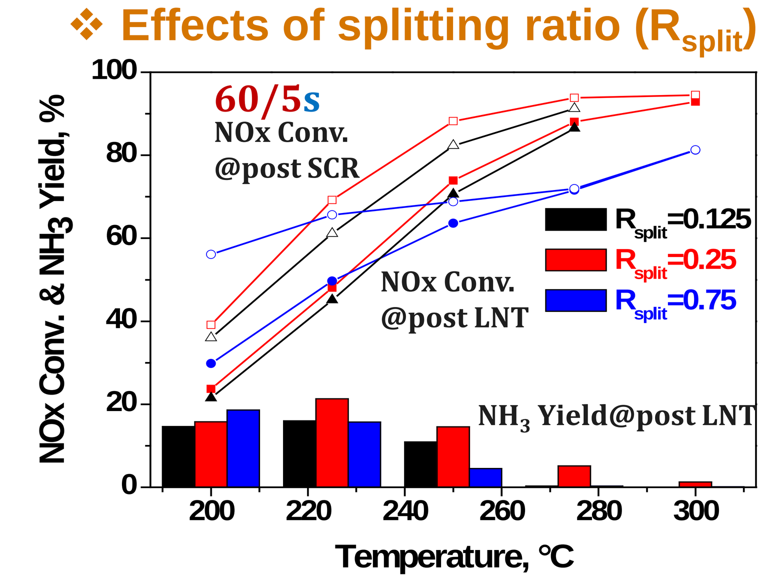
❖ Effects of cycling frequency

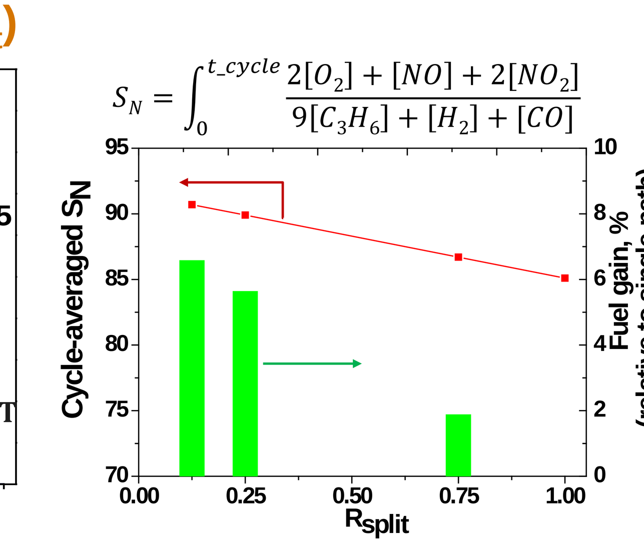
Bypass concept



- Higher cycling frequency provides higher overall NOx Conv. and NH_3 yield at the same level of fuel penalty

❖ Effects of splitting ratio (R_{split})





$$S_N = \int_0^{t\_cycle}\frac{2[O_2]+[NO]+2[NO_2]}{9[C_3H_6]+[H_2]+[CO]}$$

- Optimal R_{split} varies with operating condition and balances between fuel economy and deNOx efficiency

Summary

- Modelling analysis shows great advantages of bypass concept over the single-path, in terms of higher NOx conversion and NH_3 yield at a lower fuel penalty.
- To achieve optimal performance, multiple factors need to be taken into account, including lean/rich timing, fuel penalty, cycling frequency, non-isothermal effect, stored NOx load, and splitting ratios, etc.,

Reference

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