NO_X-chemistry modeling for coal/biomass CFD

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Contents

- Background
- NO_x-model with HCN, NH_3 and NO
- H, OH and O radical modeling
- NO solution with radical modelling
- Conclusion

Background

- Straw used to replace some of the coal in the effort to lower CO_2-emissions.
- Co-fired in suspension fired boiler with pulverized coal at the Studstrup power plant, which has 2 units of 350 MW_e each. It burns 123,150 tons of straw a year (2005).
- Earlier measurement have shown a potential for NO_X-reduction during co-firing, which is not obtained at Studstrup.
- CFD can be used to generate large amounts of data.

Chemistry in CFD

Transport equation for the mass fraction of species i

$$\underbrace{\frac{\partial}{\partial t}(\rho Y_i)}_{\text{Transient}} + \underbrace{\nabla(\rho \vec{v} Y_i)}_{\text{Convective}} = \underbrace{-\nabla \vec{J}_i}_{\text{Diffusion}} + \underbrace{R_i + S_i}_{\text{Source}}$$

Net source of i due to chemical reaction

- Mixing limited
- Reaction rate limited

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NO_X models

De Soete (1975)	Lars Storm Pedersen (1998)	Glarborg (2004)
2 reactions (4 with NH_3 and HCN)	36 reactions	509 reactions
3 species solved for	3 species solved for	73 species solved for
O_2 must be known	H, O, OH, H_2O, O_2, H_2, CO and CO_2 must be known	-

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LSP NO_x-model

- NO_x-model by Lars Storm Pedersen
  - Based on 36 reactions
  - 3 active species NO, HCN and NH_3
  - 8 steady state species CN, HOCN, HNCO, NCO, NH_2, NH, N and N_2
  - Reaction rates for NO, HCN and NH_3 all become complex algebraic functions
    - $R = f(NO, HCN, NH_3, H, O, OH, H_2O, O_2, H_2, CO, CO_2, N_2)$

H, O, OH:

- Not easily obtainable through the flowfield/combustion solution
- Can be estimated from the main species using steady-state and partial equilibrium assumption

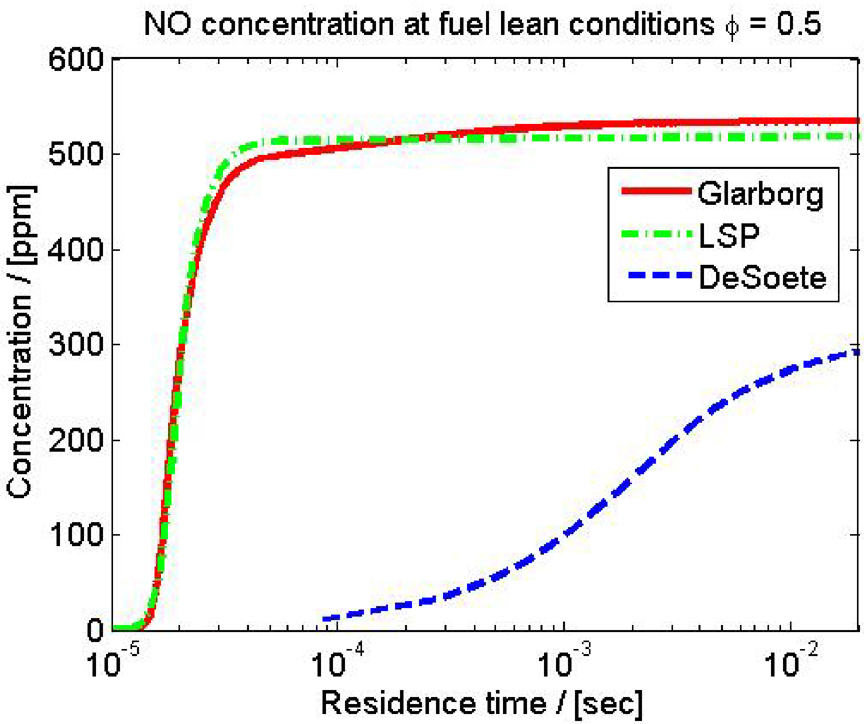
$H_2O, O_2, H_2, CO, CO_2, N_2$:

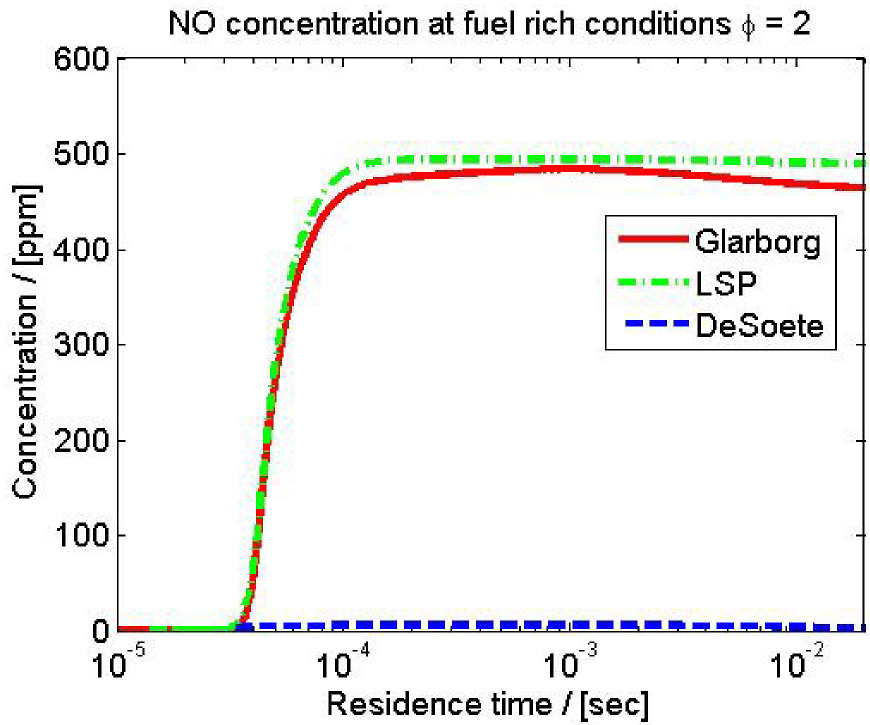
- Obtainable through the flowfield/combustion solution

Plug flow reactor simulations

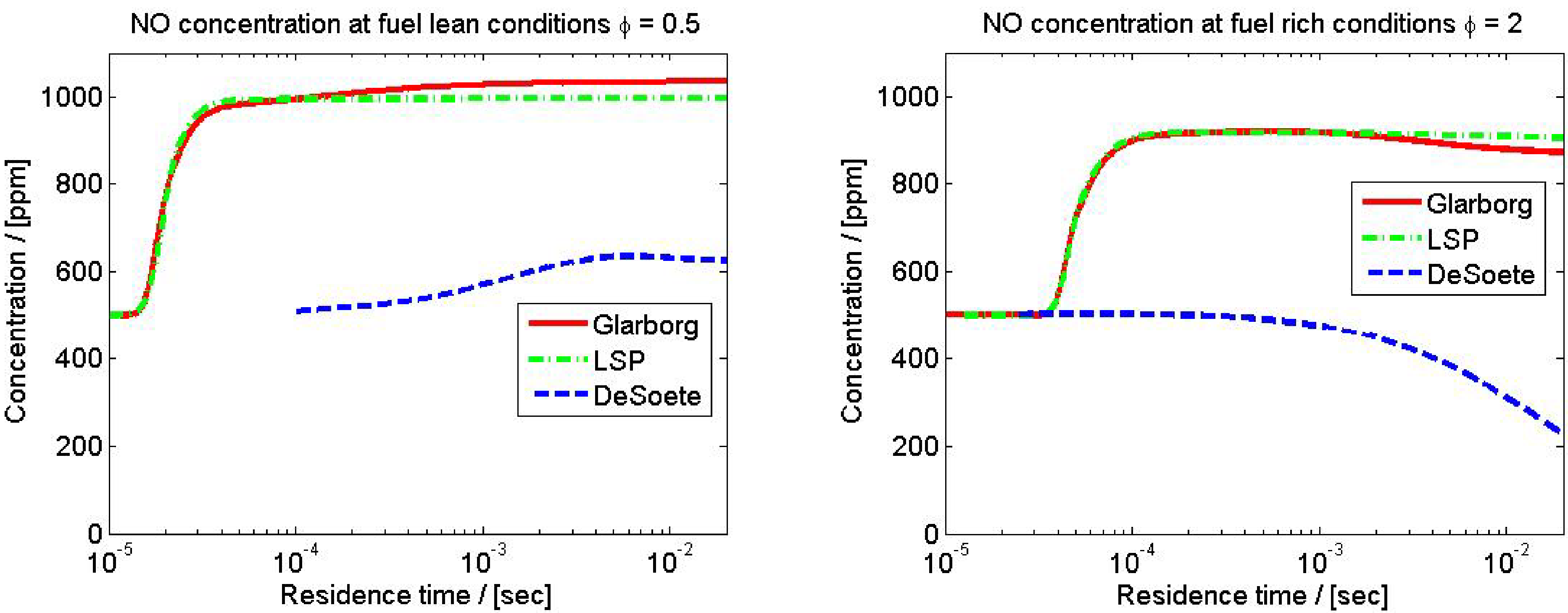
- Major species
  - $[H_2] = [CO] = 4$ vol%
  - $[H_2O] = [CO_2] = 6$ [vol%]
- Minor species
  - $[NH_3] = 200$ ppm
  - $[HCN] = 300$ ppm
- Temperature 1800 K

[NO] at different residence times. With initial [NO] = 0 ppm.





[NO] at different residence times. With initial [NO] = 500 ppm.



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Advantages/Disadvantages with the LSP model

- Advantages:
  - Reacts as fast as the complex model. De Soete reacts slower.
  - NO levels comparable to complex model. De Soete is off especially at fuel-rich conditions.
- Disadvantages:
  - Knowledge of H_2O, O_2, H_2, CO and CO_2 required. De Soete requires only $O_{2.}$
  - The LSP model requires knowledge of H-radicals.

Contents

H-radical models

- 8 reactions
- 3 major species O_2, H_2 and H_2O
- 3 radical species H, O and OH

1	$H + H + M = H_2 + M$
2	$H + OH + M = H_2O + M$
3	$H + O + M = OH + M$
4	$O + O + M = O_2 + M$
5	$OH + OH = H_2O + O$
6	$O + OH = H + O_2$
7	$O + H_2 = OH + H$
8	$OH + H_2 = H_2O + H$

- 4 solutions suggestions:
  - **Partial:** H, O and OH from partial equilibrium of reaction 1, 4 and 5
  - **H-steady:** H in steady state, O and OH from partial equilibrium of 4 and 5
  - **H&O-steady:** H and O in steady state, OH from partial equilibrium of 5
  - **H&O&OH-steady:** H, O and OH in steady state.

Solutions

- Partial:

$$[H] = \sqrt{\frac{C}{K_1} \cdot [H_2]} \qquad [O] = \sqrt{\frac{C}{K_5} \cdot [O_2]} \qquad [OH] = \sqrt{\frac{1}{K_6} \cdot [H_2O] \cdot \sqrt{\frac{C}{K_5} \cdot [O_2]}}$$

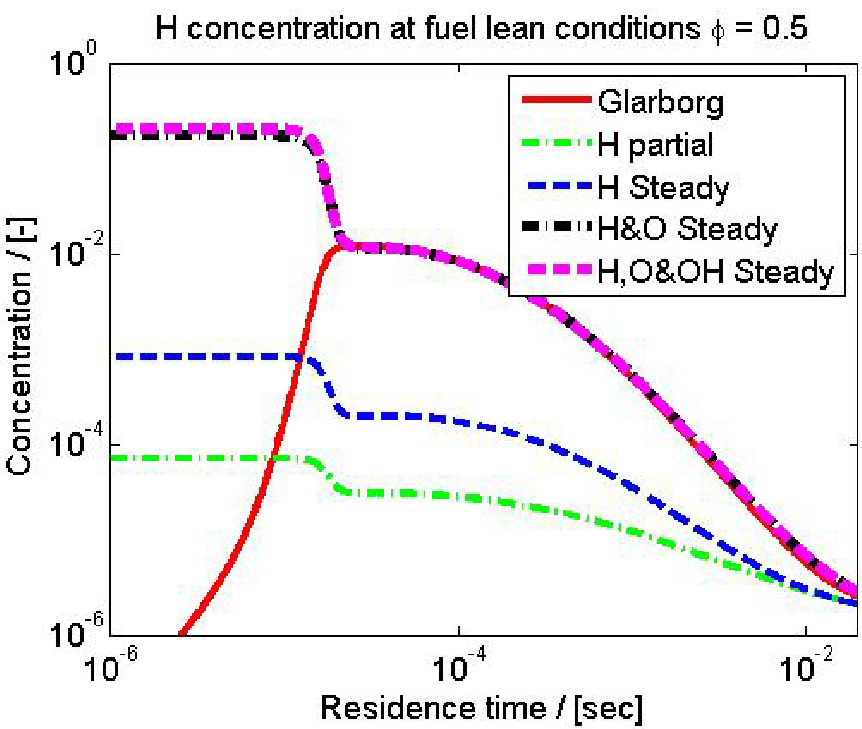
- H-Steady:

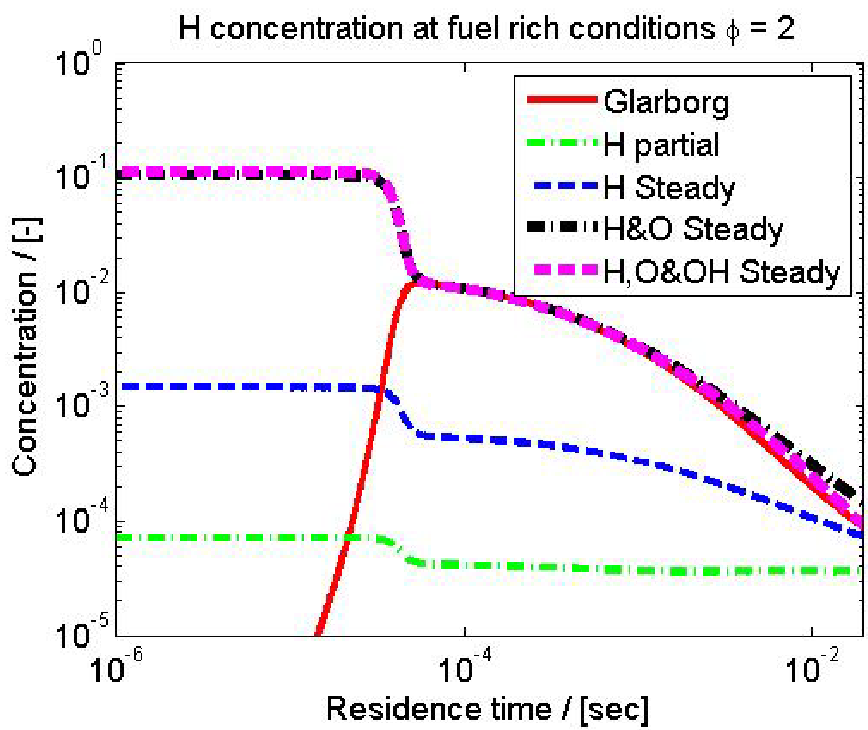
$$[H] = \frac{-b + \sqrt{b^2 - 4 \cdot a \cdot c}}{2 \cdot a}$$

where a, b and c are functions of O, OH, O_2, H_2, and H_2O. O and OH are found as in Partial

- H&O-Steady:
  - Solved numerically. Two nonlinear equations with two unknowns.
- H&O&OH-Steady:
  - Solved numerically. Three nonlinear equations with three unknowns.

[H] at different residence times





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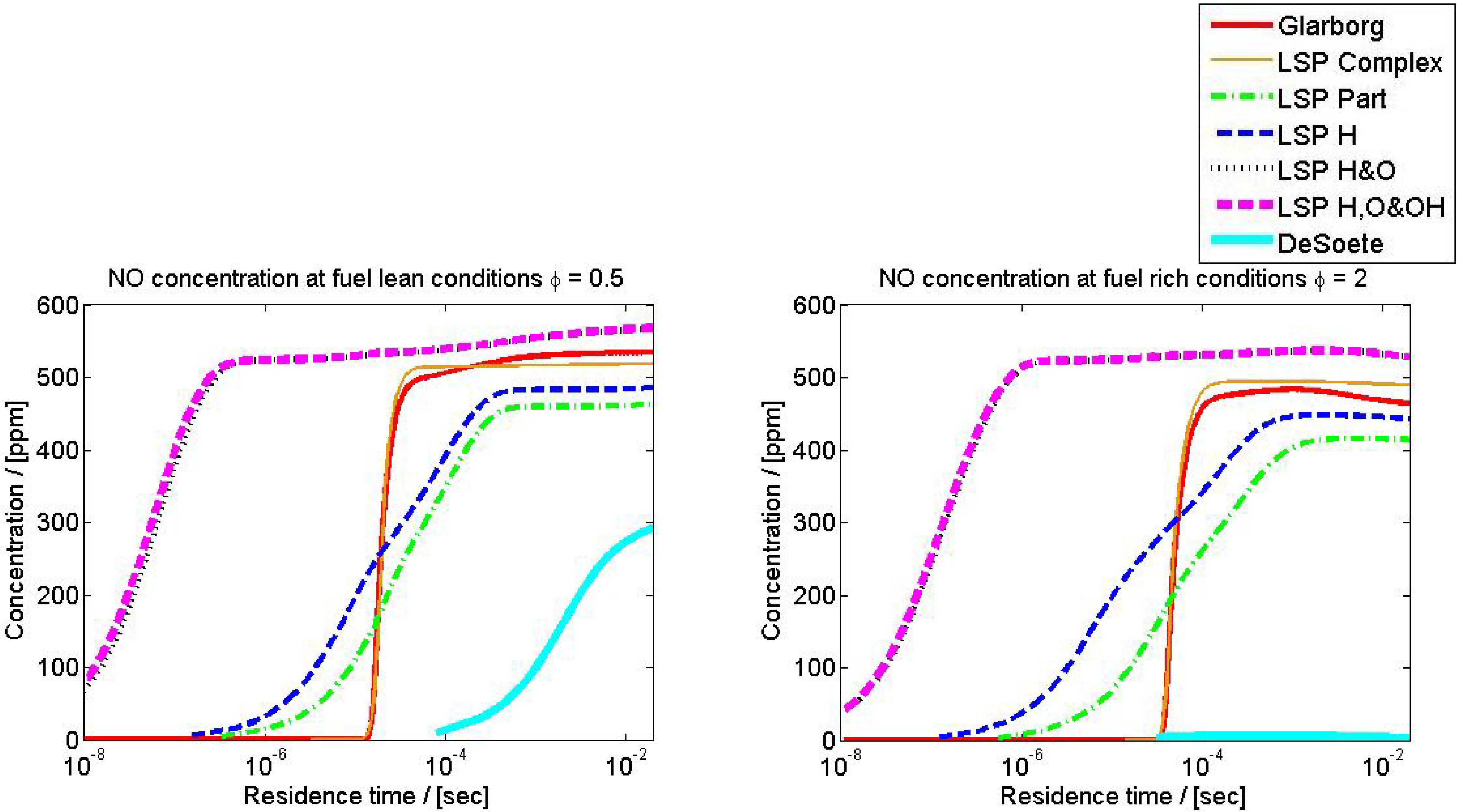
[NO] at different residence times. With initial [NO] = 0 ppm.



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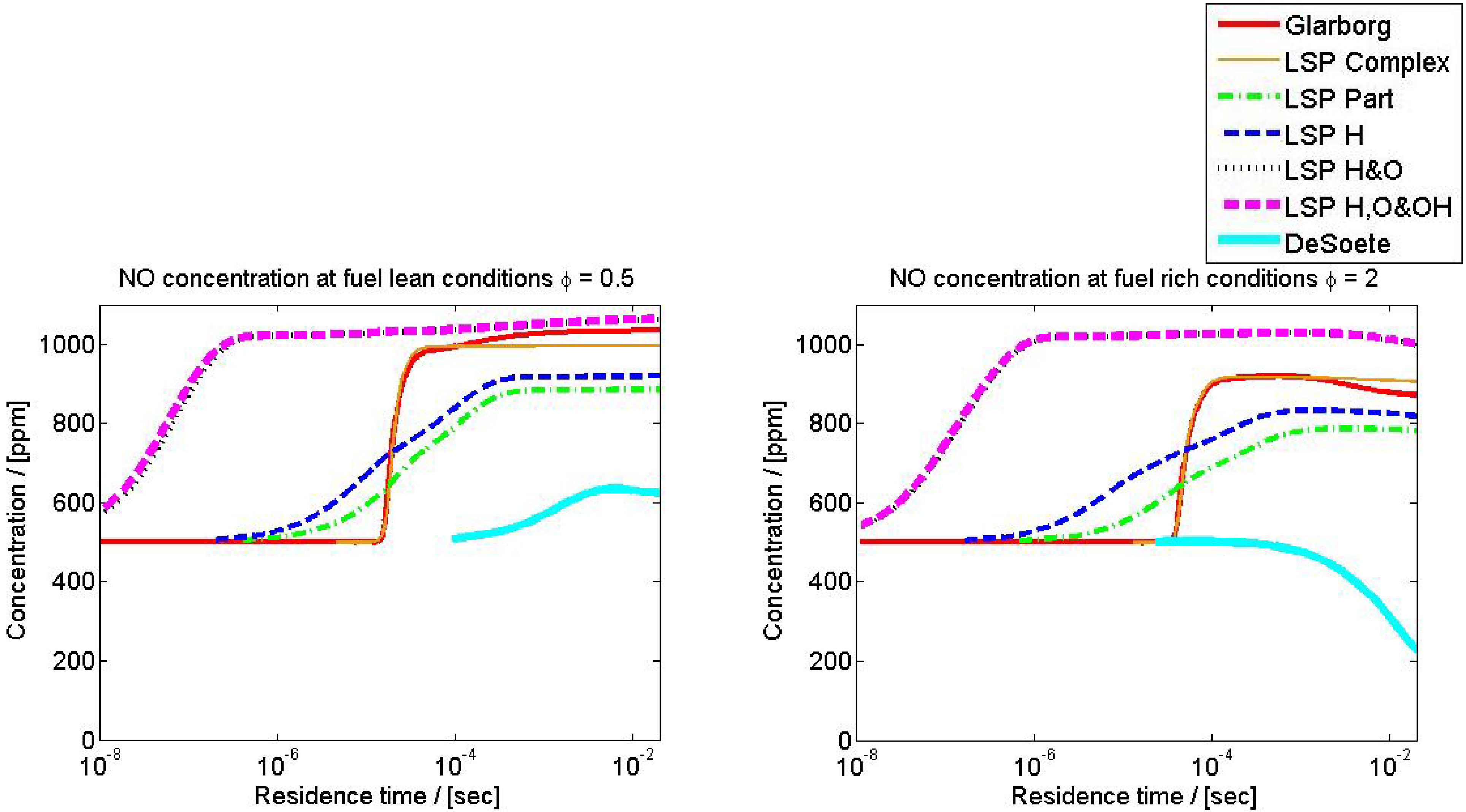
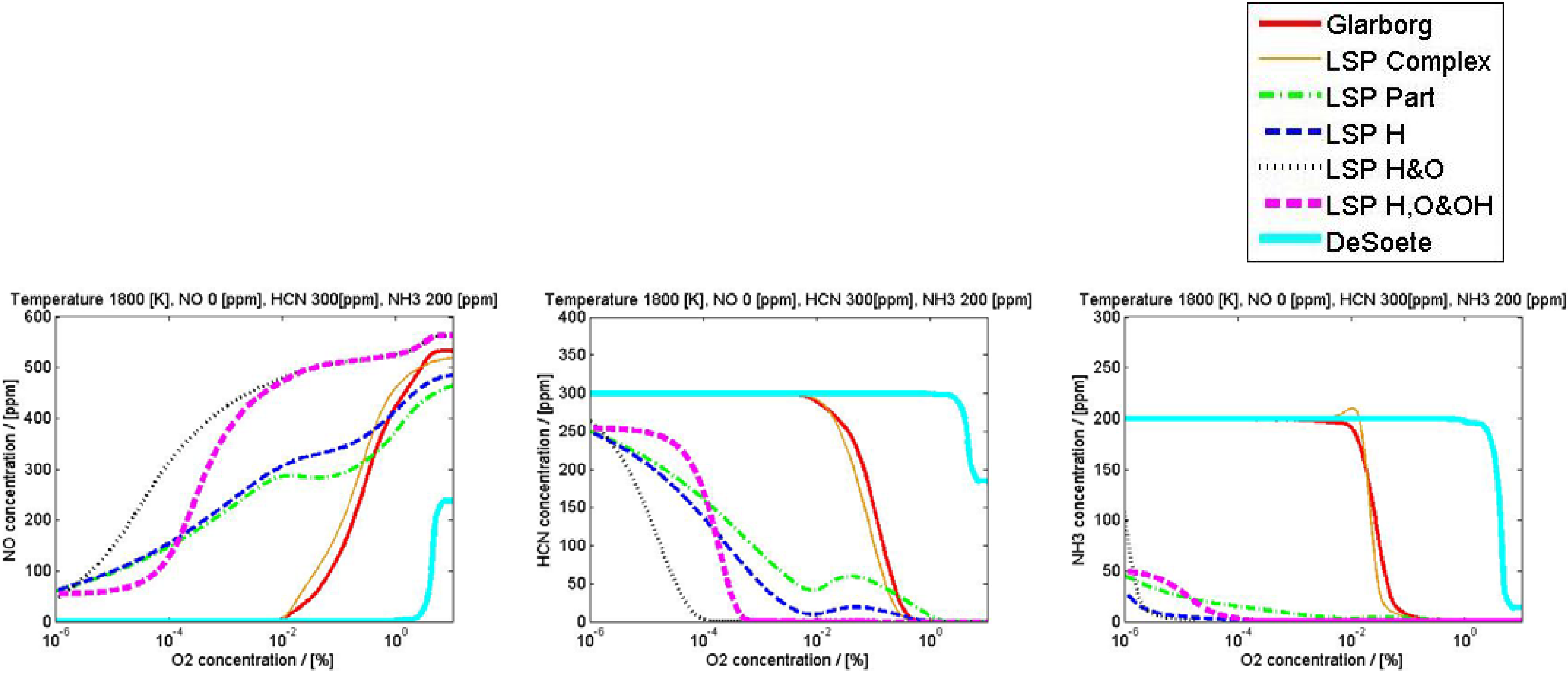
[NO] at different residence times. With initial [NO] = 500 ppm.



Nitrogen species after 5 msec as a function of O_2. [NO] = 0 ppm

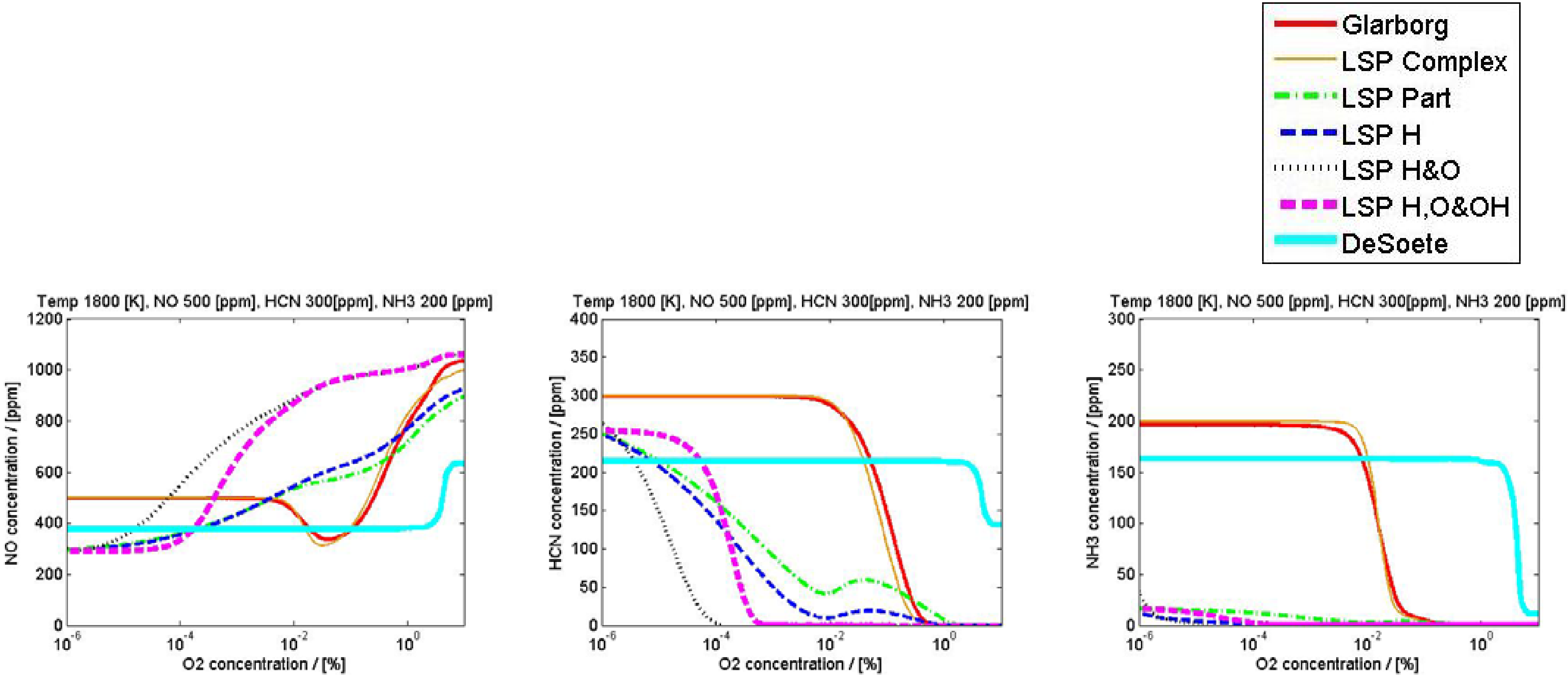


NO

HCN

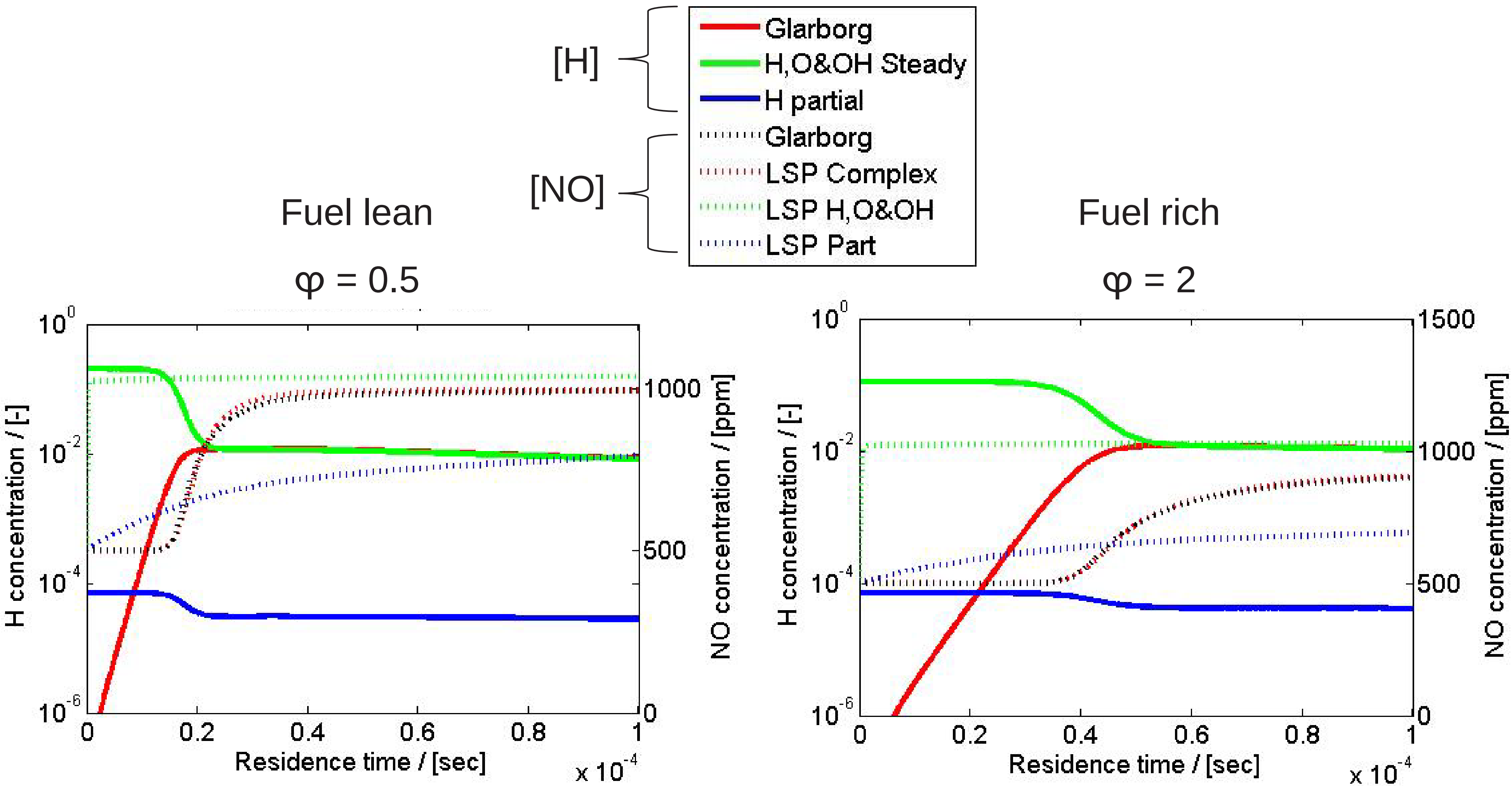
NH3

Nitrogen species after 5 msec as a function of O_2. [NO] = 500 ppm



NO HCN NH3

[NO] and [H] at different residence times



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Conclusion

- The H, O and OH steady state model mimic the Glarborg model best.
- The NO_X-model has the potential to give results similar to those of Glarborg.
- NO_X-model with radical models
  - Over predicts speed
  - Over predicts NO creation/destruction under very fuel rich conditions
- The partial equilibrium model does best with the NO_X-model.
- The models do better than De Soete.