Journal of Zhejiang University-SCIENCE A (Applied Physics & Engineering)

Cite this as: Xu-bo GAN, Dong-wei YAO, Feng WU, Jia-wei DAI, Lai WEI, Xing-wen LI, 2016. Quasi 1D modeling of two-phase flow and deposit formation for urea-selective catalytic reduction systems. *Journal of Zhejiang University-SCIENCE A (Applied Physics & Engineering)*, 17(8):597-613. http://dx.doi.org/10.1631/jzus.A1500303

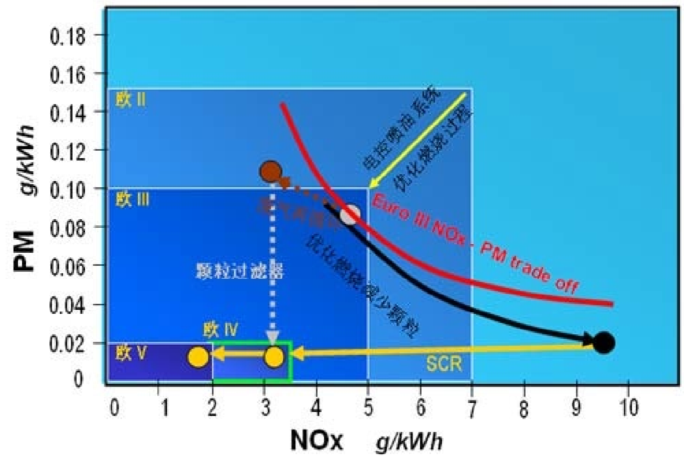
Quasi 1D modeling of two-phase flow and deposit formation for urea-selective catalytic reduction systems

Xu-bo GAN

浙江大學

Institute of Power Machinery and Vehicular Engineering,
Zhejiang University

Introduction

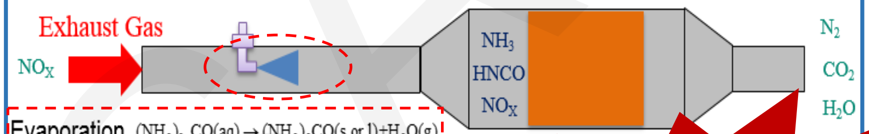


SCR is one of the most promising methods to reduce NOx emission from heavy-duty vehicles

Hydrolyiss $HNCO(g)+H_2O \rightarrow NH_3(g)+CO_2(g)$

Standard SCR $4NH_3+4NO+O_2 \rightarrow 4N_2+6H_2O$

Fast SCR $4NH_3+2NO+2NO_2 \rightarrow 4N_2+6H_2O$



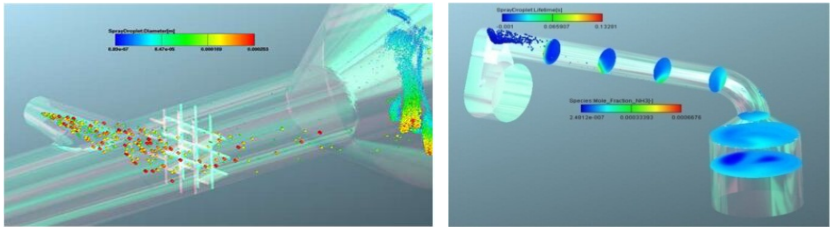
Evaporation $(NH_2)_2CO(aq) \rightarrow (NH_2)_2CO(s\ or\ l)+H_2O(g)$

Thermolysis $(NH_2)_2CO(s\ or\ l) \rightarrow NH_3(g)+HNCO(g)$

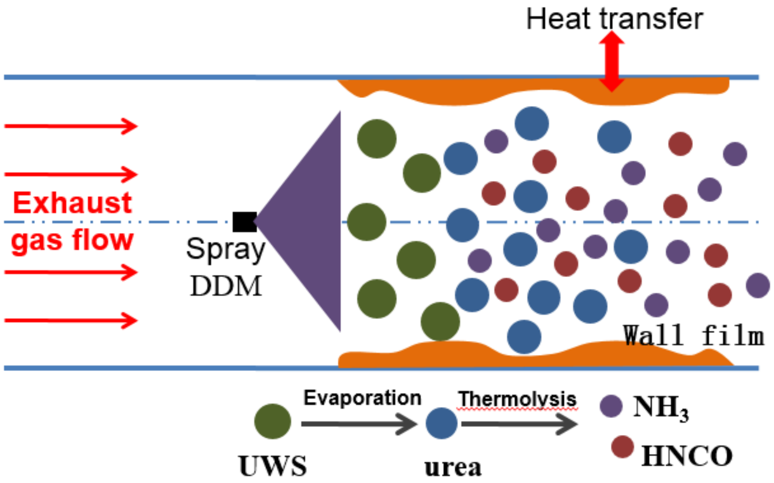
Urea injection process is very important for SCR performance

Urea deposits

Injection strategy & ammonia production



Modeling Method



- Gas flow

$$\frac{\partial \rho_g}{\partial t}+\frac{\partial \rho_g u_g}{\partial x}=0 \qquad \frac{\partial \rho_g H_g}{\partial t}+\frac{\partial \rho_g u_g H_g}{\partial x}=\alpha_{gw}(T_w-T_g)a_{geo}+S_{qgs}$$

$$\frac{dP_g}{dx}=-K_d u_g \qquad \frac{\partial \rho_g w_{i,g}}{\partial t}+\frac{\partial \rho_g u_g w_{i,g}}{\partial x}=S_{species}$$

- Heat transfer of pipe wall

$$\frac{\partial}{\partial t}(T_w \rho_{l,w} c_{p,l,w})=\frac{\partial}{\partial z}(\lambda_{l,w}\frac{\partial T_w}{\partial z})+\frac{1}{r}\frac{\partial}{\partial r}(r\lambda_{l,w}\frac{\partial T_w}{\partial r})+S_{wd}+S_{wf}$$

$$\frac{\partial T_w}{\partial z}=0 \quad @\ z=0 \qquad \frac{\partial T_w}{\partial r}=-\frac{\alpha_{gw}}{\lambda_{l,w}}(T_g-T_w) \quad @\ \mathrm{r}=\mathrm{r}_{\mathrm{gw}}$$

$$\frac{\partial T_w}{\partial z}=0 \quad @\ z=\mathrm{L}_{\mathrm{pipe}} \qquad \frac{\partial T_w}{\partial r}=-\frac{\alpha_{wa}}{\lambda_{l,w}}(T_w-T_{amb}) \quad @\ \mathrm{r}=\mathrm{r}_{\mathrm{wa}}$$

- Liquid phase model

(droplet motion、evaporation、thermolysis)

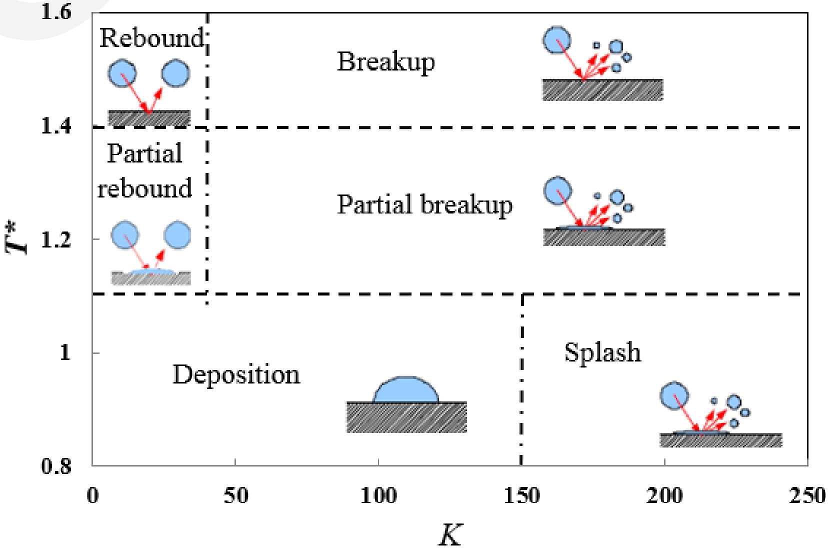
$$\frac{dm_d}{dt}=-\pi D_d \rho_{g,mix}\Gamma_{ref} Sh \ln(1+B_M)\times(T_\infty/673) \qquad \frac{du_d}{dt}=\frac{3}{4}\frac{\rho_g}{\rho_d}\frac{C_d}{D_d}\left|u_g-u_d\right|(u_g-u_d)$$

$$\frac{dT_d}{dt}=\frac{(-dm_d/dt)c_{p,vap}(T_g-T_d)/B_T-L_{vap}}{m_d c_{p,d}} \qquad \frac{dm_d}{dt}=-m_d A e^{(-Ea/RT_d)}$$

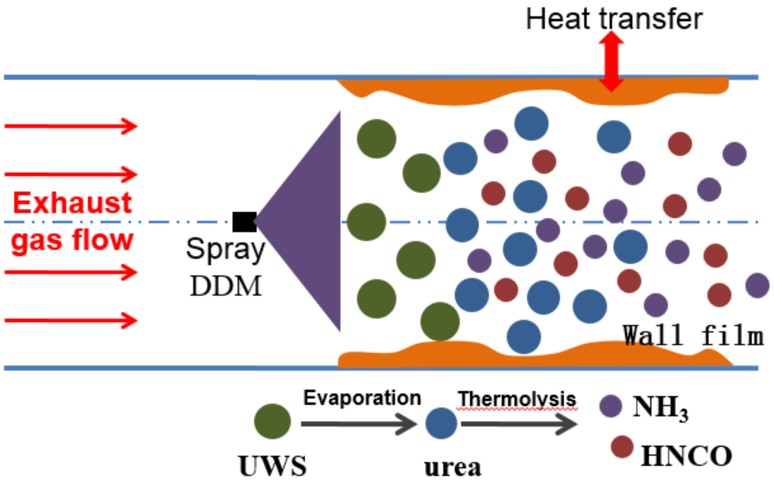
- Spray wall interaction

$$s_{\mathrm{d}}=\left|\int u_{\mathrm{r}} dt\right| \geq d_{\mathrm{c}}$$

$$K=\frac{(\rho D)_{\mathrm{d}}^{0.75} u_{\mathrm{d}}^{1.25}}{\sigma_{\mathrm{d}}^{0.5}\mu_{\mathrm{d}}^{0.25}} \qquad T^*=\frac{T_{\mathrm{w}}}{T_{\mathrm{sat}}}$$



Wall film model



- Wall film thickness

$$\delta_i = \frac{V_{\mathrm{f},i}}{a_i}$$

- Wall film motion

$$F = (u_\mathrm{g} - u_\mathrm{f})\delta f_i$$

- Wall film evaporation

$$\frac{dm_\mathrm{f}}{dt} = -a_\mathrm{f} Y_\mathrm{w} \rho_\mathrm{g} h_\mathrm{m} \ln(1 + B_\mathrm{m})\beta(\frac{T_\mathrm{w}}{T_\mathrm{sat}})^2$$

- Wall film thermolysis

	Reactions
R1	urea→NH_4^++NCO^-
R2	NH_4^+→NH_3(g)+H^+
R3	NCO^-+H^+→HNCO(g)
R4	urea+ NCO^-+H^+→biuret
R5	biuret→urea+ NCO^-+H^+
R6	biuret+ NCO^-+H^+→CYA+NH_3(g)
R7	CYA→3NCO^-+3H^+
R8	CYA+ NCO^-+H^+→ammelide+CO_2
R9	ammelide→2NCO^-+2H^++HCN(g)+NH(g)

- Continuity equation

$$\frac{\partial A_\mathrm{s}}{\partial t} + \frac{\partial A_\mathrm{s} u_\mathrm{f}}{\partial x} = \frac{S_\mathrm{m} Y_\mathrm{u}}{M\theta}$$

Active surface

$$\frac{\partial m_\mathrm{f}}{\partial t} + \frac{\partial m_\mathrm{f} u_\mathrm{f}}{\partial x} = S_\mathrm{m} + S_\mathrm{th} + S_\mathrm{eva}$$

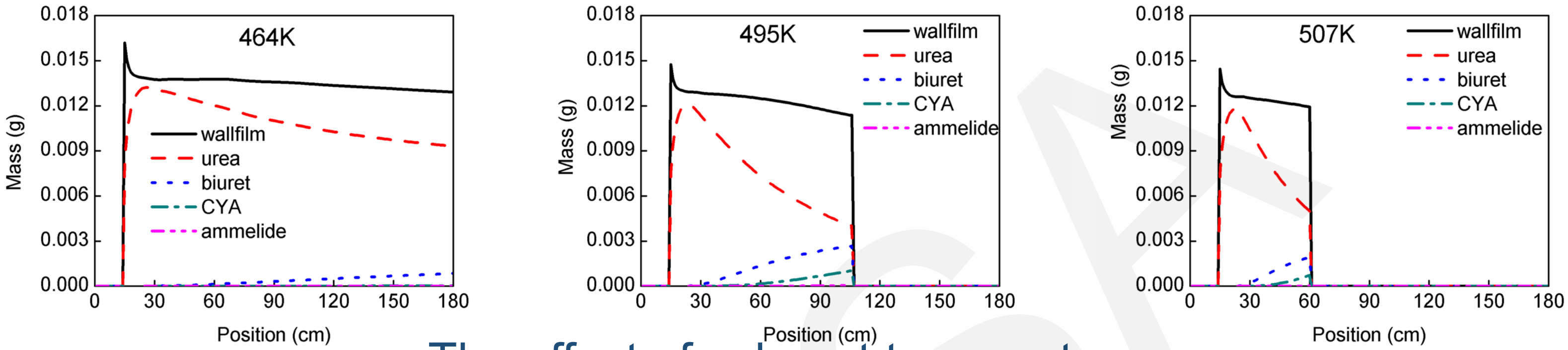
Film mass

$$\frac{\partial m_i}{\partial t} + \frac{\partial m_i u}{\partial x} = S_i$$

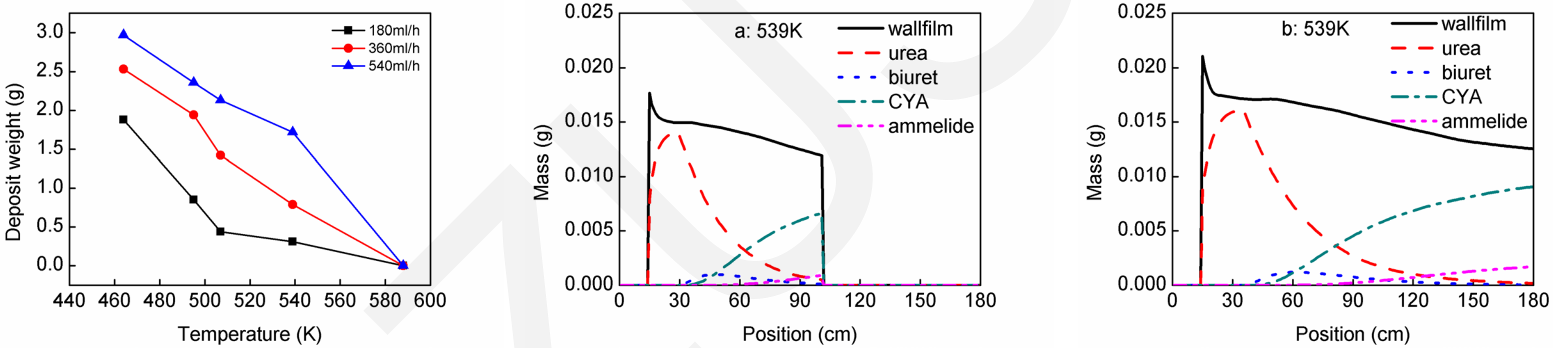
Species mass

A new one dimensional wall film model simplified from a three dimensional model is proposed. The model assumes that the wall film distributes evenly on the inner surface of the pipe mesh

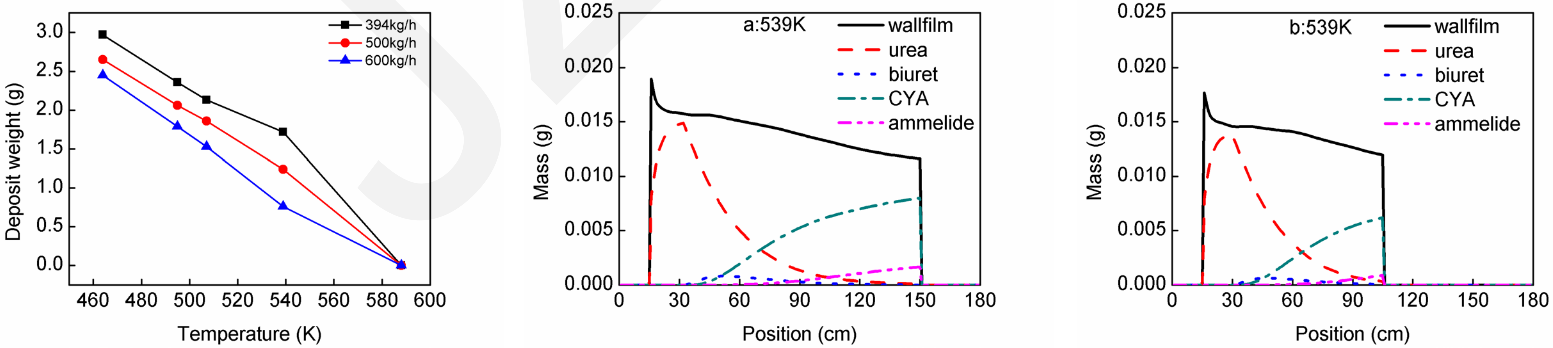
Results and discussion



The effect of exhaust temperature



The effect of UWS injection rate



The effect of exhaust mass flow

Conclusions

- A simplified one dimensional model of gas-liquid two phase flow is presented. The developed model can calculate not only the generation of the reducing agent but also the formation of deposits in the exhaust pipe.

- A combination of Birkhold's direct decomposition model and Ebrahimian's kinetic model was implemented, and a new one dimensional wall film model was developed. The position, weight and components of deposits can be simulated.

- Simulation results showed that: (1) A decrease in exhaust temperature will increase the wall film region and weight of deposits. (2) Deposit components are highly dependent on temperature: when the temperature is low, most deposits are urea, but when the temperature rises, by-products such as biuret and CYA begin to form. (3) The UWS injection rate can affect the total mass of wall film and expand the film region, but it has little influence on deposit components. (4)An increase in exhaust mass flow can decrease the total weight of deposit and the film region on the pipe wall because of the promotion of the mass and heat transfer process both in the droplets and wall film.