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General Background
The information below and in the attached MatLab program files are made available through the Crosscut Lean Exhaust Emissions Reduction Simulation (CLEERS) website as supplemental supporting documentation concerning previously published research results from the Fuels, Engines, and Emissions Research Group at the Oak Ridge National Laboratory. Funding for this research was provided by the U.S. Department of Energy Office of Freedom Car and Vehicle Technologies under the Energy Efficiency and Renewable Energy Program. The associated files are intended for research and discussion purposes only and are not warrantied for any other purpose, express or implied.

In posting this collection of computer codes, our objective is to provide an example set of computational tools that potentially could be useful for evaluating and summarizing observed trends in laboratory bench reactor characterization measurements of lean NOx trap (LNT) materials. UNDER NO CIRCUMSTANCES ARE THESE CODES INTENDED FOR FULL LNT SYSTEM SIMULATIONS OR SYSTEM DESIGN! For this reason, there are a considerable number of simplifying assumptions that are made, and these assumptions are documented in the accompanying files that can be downloaded from the CLEERS website. It is our intention to post improvements to these codes from time to time as they become available, and any updates will be documented as update and/or version information at the beginning of each function file. Future improvments that are currently planned include graphical user interfaces for defining input conditions and parameters and displaying results, as well as improvement in the physical assumptions made.

The code files are structured to run in a linked fashion to simulate the time and spatial species and temperature variations in an LNT monolith during a defined sequence of capture and regeneration cycles. To function properly, all of the associated function files should be located in the same directory. IN addition to defining the cycle conditions, it is necessary for the user to specify initial conditions, flow and geometric parameters for the monolith, and isotherm and kinetic rate coefficients. Example default values are provided in the current files, but these should be adjusted by the user to conform to their specific conditions and LNT material properties.

Any questions regarding the technical details of the model or LNT behvaior should be directed to Kalyana Chakravarthy at ORNL (chakravartvk@ornl.gov). General questions concerning CLEERS should be directed to Stuart Daw (dawcs@ornl.gov). Questions related to MatLab or the CLEERS website should be referred to Vitaly Prikhodko (prikhodkovy@ornl.gov) .

Specific information regarding the program files is given below. The program code is divided into explicit MatLab functions, each of which is intended to perform specific calculations associated with various steps in the function of lean NOx traps materials. Each of these functions is described along with its input and output arguments. Explicit comments are also provided in each code file.

Global LNT model :
Note: This is the main function routine that coordinates all other functions.
- Tracks total NOx during capture and regen
- Concentration of O2 and reductant compared locally to decide between capture and regen
- NOx storage limited by i) BL mass transfer & ii) internal mass transfer
- No reductant during lean-phase
- Track single reductant species during regen
- Max. Regeneration rate limited by reductant mass transfer to the surface
- NOx released into bulk flow during regeneration assumed to be NO for computing the regeneration stiochiometry (i.e., the consumption rate of reductant)
  NOx can be stored in nitrate or nitrite forms (matters while determining

the reductant consumption rate)
- Kinetics at a given location lag the temperature by one time-step

User specified inputs :

Inflow : Start and end time for the simulation
engine-out NOx, reductant, O2, velocity/flowrate,temperature, pressure with time

Initial conditions : Spatial-profiles of Gas-phase and surface concentrations of NOx, reductant (default : 0 mol/m3 for all quantities)
Gas-phase O2 concentration (default : 0 mole/m3)
Nitrate/nitrite loading profile (default : 0 mol/m3)
Gas and surface temperatures (default : 300C)
pressure (default : 1 atm)

isotherm-inv : provides surface/wall NOx conc given surface temperature & nitrate loading

isotherm_slope: rate of change of NOx storage with surface NOx concentration at equilibrium at given surface NOx concentration & surface temperature

heat_release_parameters : heat release for the release and reduction reactions

All regeneration properties specific to a given reductant. In case of multiple reductant, corresponding weighted average quantities need to be used.

Cat. Specifications : variables used in the code are indicated in brackets

Isotherm : NOx conc (ppmNOx) vs. stored NOx (NOx_storage)

capacity : temperature (temperature_storage) vs. relative capacity (temperature_scaling)

NO2- fraction : temperature (temperature_storage) vs. nitrite fraction (nitrite_fraction)

Stored NOx can
- desorb under neutral conditions (no NOx/O2) at a prescribed desorption rate
- be released at a prescribed release rate
- reductant requirement for release determined by nitrite/nitrate fractions

Releases NOx can
- be reduced to N2
- enter the bulk gas

Desorption rate, release and reduction rates are specified at functions of temperature

Internal rate limiting storage : determined by 3 parameters

rate_parameter3 : Initial rate of storage
rate_parameter1 : ratio of terminal to initial rates of storage
rate_parameter2 : characterizes the exponential decrease of the rate with NOx storage

rate_int = rate_parameter3*[rate_parameter1 + (1-rate_parameter1)*exp(-rate_parameter2*q)]