CLEERS Databases for Aftertreatment Modeling

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Acknowledgments

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Databases Needed

- Engine databases
- Aftertreatment device databases
- Kinetics databases

- Major components needed in databases:
  - Experimental results
  - Models

Engine Databases

- Types of engine databases
  - Type 1: Exhaust valve out values for FTP cycle
  - Type 2: Exhaust valve out values for constant speed runs
  - Type 3: GT-Power files for specific engines
- Detailed description of hardware
  - Engine specifics (model, modifications, history, etc.)
  - Measuring equipment description
- Operating condition details
  - Flow rates, fueling rates, inlet/ambient conditions, rpm, load, EGR, boost, coolant conditions, etc.
  - Composition, temperature at aftertreatment device location (if available)

Aftertreatment Device Databases

- Types of device databases
  - Measurements from catalytic reactor runs
    - Temperatures, flow rates and compositions
- Description of device
  - Model/serial number, geometric specifications
  - Catalyst material
  - Aging history
  - Measuring equipment description
- Operating condition details
  - Emission source
  - Device heating, regeneration details, etc.
  - Steady or un-steady operation specifics

Kinetics and Reaction Databases

- Types of kinetics/reaction databases
  - Species properties in Chemkin input format
    - Thermodynamic properties
    - Transport properties
  - Kinetic mechanisms for specific catalytic devices
    - Global mechanisms for total device
    - Mechanisms for specific aspect of catalyst process
    - Chemkin format
- Description of device
  - Composition, geometry, etc.
- Operating condition details
  - Standard operating condition ranges, etc.

Targeted Software Tools (1)

- GT-Power
  - For full engine/powertrain modeling
  - Needs aftertreatment device models
  - Needs better exhaust emissions models

- Chemkin Package
  - For single channel detailed kinetic modeling
    - 3-way catalysis, NOx absorber, SCR
  - Difficulty: detailed kinetic mechanisms are difficult to obtain and use

Targeted Software Tools (2)

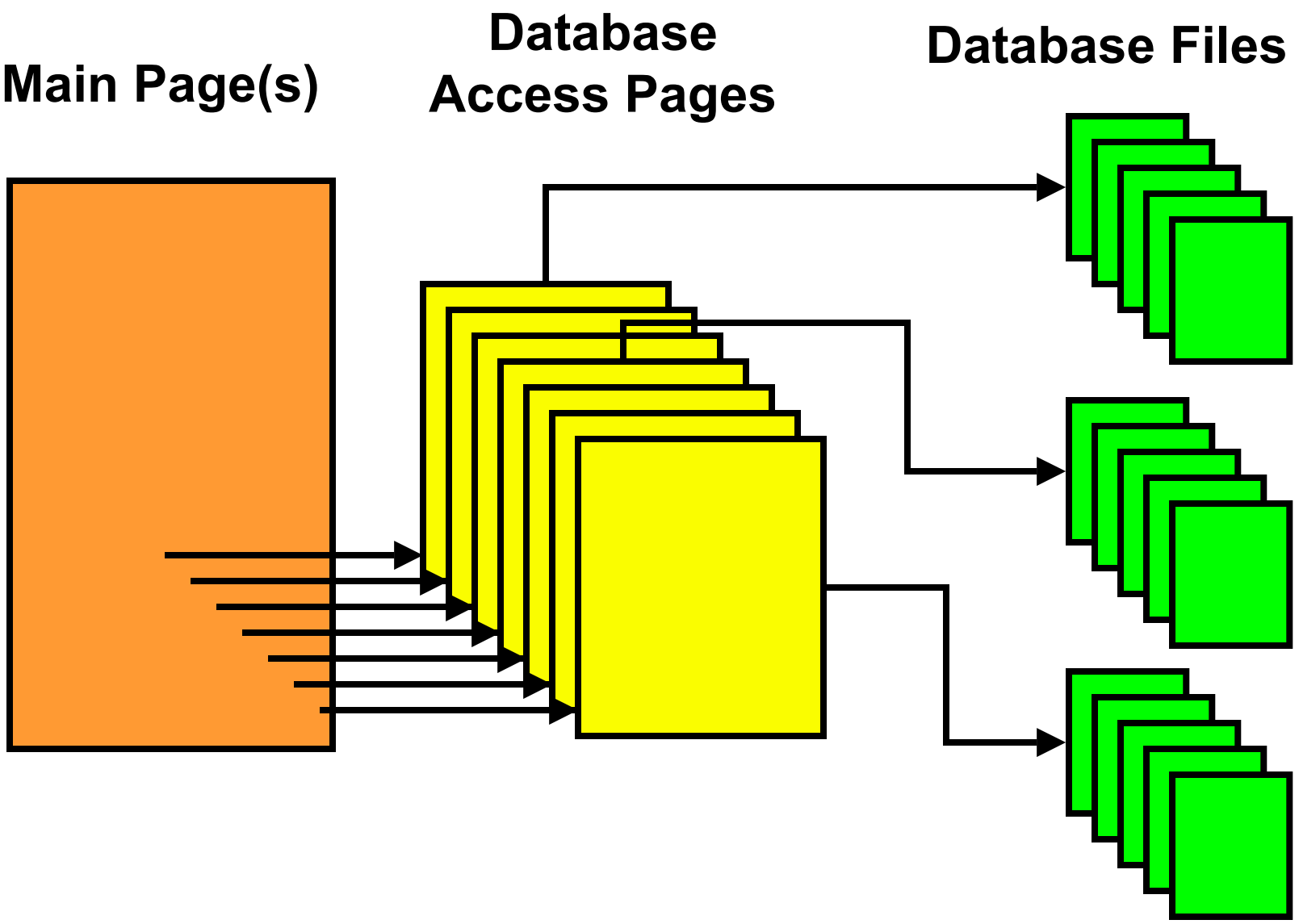
- Matlab/Simulink
  - Industry standard modeling tool
  - Lacks wave-dynamics and typical engine components
  - Integration with GT-Power is currently one-way, but better coupling is in the works
- Advisor/PSAT
  - Powertrain modeling tool (uses Matlab/Simulink)
  - Focus is on HEV, not emissions or diesels
- Fluent and/or Star-CD
  - For 3D flow modeling
    - Manifolds, device inlets, etc.
    - Composition and thermal distribution
  - Lack appropriate detailed kinetics

Device Models

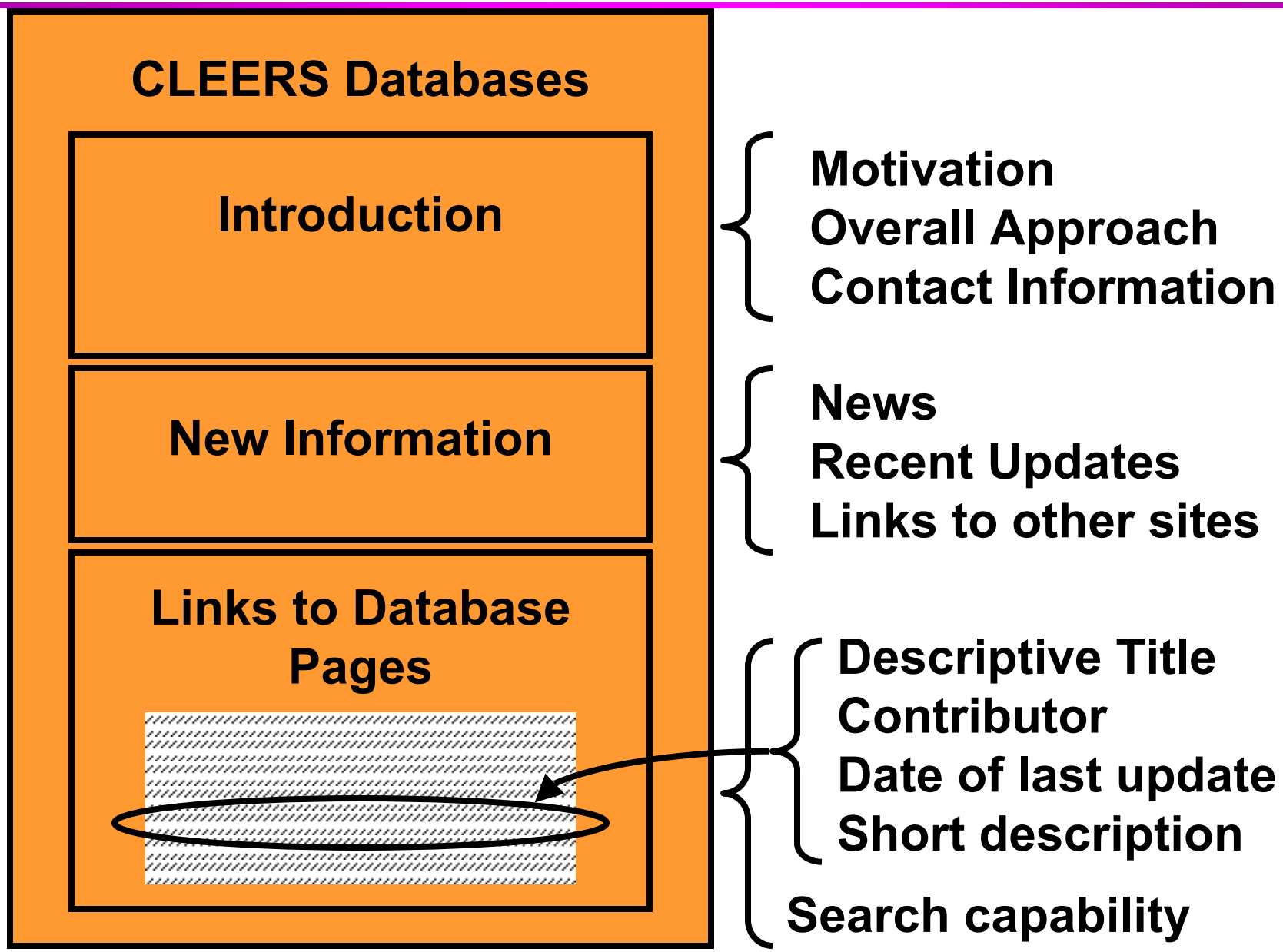
- Major aftertreament device models needed
  - Diesel particulate filter
  - 3-way catalyst
  - NOx absorber
  - SCR
  - Hydrocarbon absorber model

- Engineering tools
  - Single (or bulk) channel, global kinetics
  - Include thermal characteristics
  - Fast (integrate into system simulations)
  - Tunable coefficients to match experimental data

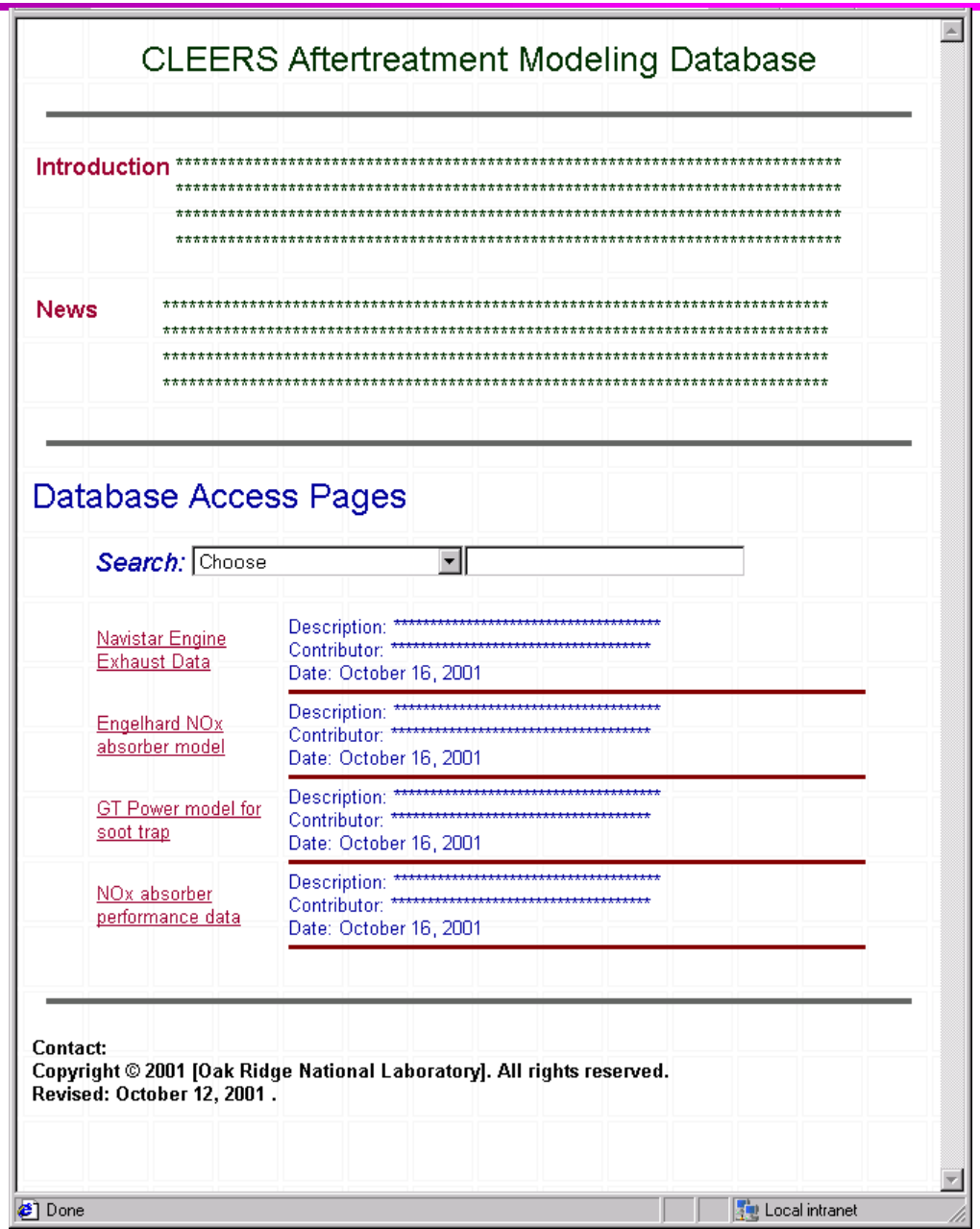
CLEERS Aftertreatment Website Structure

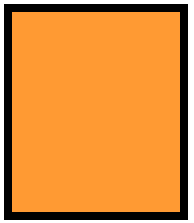


Main Page of Database Website



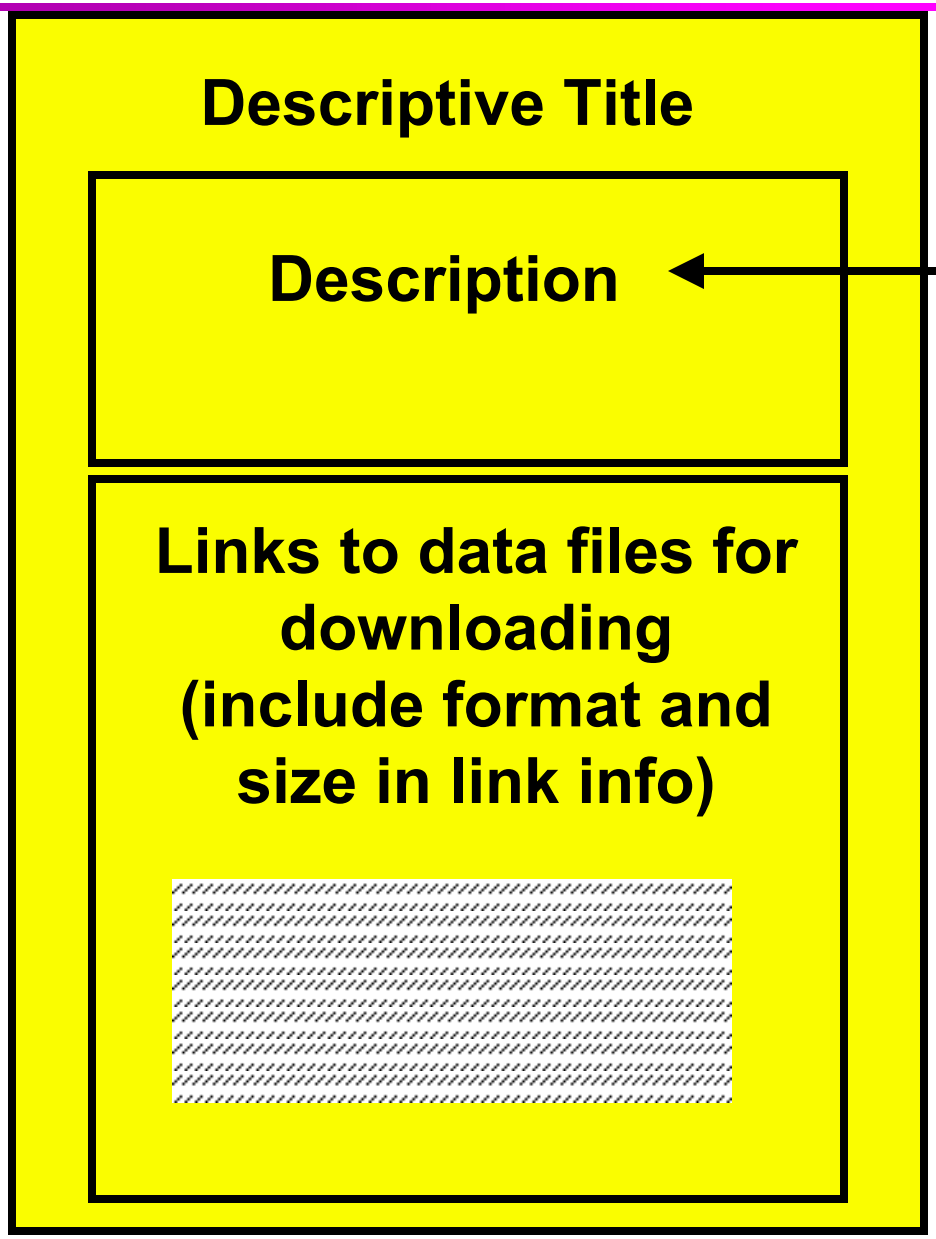
Example CLEERS Database Main page





- Flat database
  - Access pages
- Include information about contributing to database

Typical Database Access Page



- Overview
  - Device, operating conditions, type of data
- Submitter and contact information
- Detailed description of files
  - Naming convention
  - File types (text, xls, etc.)
  - File sizes
  - File contents
    - Include units
  - Format of data in file
    - Sample code for reading files

Example Data Access Page

Engelhard NOx Absorber Model No. 1

General Description

****
****
****
****

Specific Information

- Model number: *****
- Description of device modeled: **********
****
****
- Model assumptions: **********
- Detailed model description: (Link to another page)
- Instructions for using the model: **********
****
- Sample results: (Link to another page)
- Model application software: GT Power
- Contact Information: **********

Files

Engelhard NOx Absorber Model 1

- File name: **********
- File format: GT Power
- File size: **********
- Date: **********

Test data for NOx Absorber Model 1

- File name: **********
- File format: Text, 3 header lines, 4 columns of data
- File contents: Temperature (K), flow rates (m/s), *******
- File size: **********
- Sample code for reading file:

```
c read header lines
      do i = 1,3
        read (input_file,*)
      end do
c read data
      do i = 1,312
         read(input_file,9000) temp,mdot,***,***
      end do
9000  format(4e15.5)
```

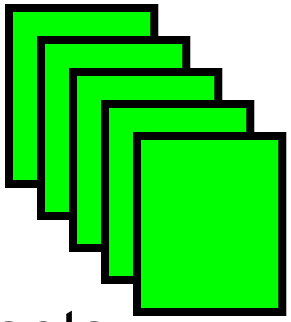
- Date: **********

Contact:

Revised: October 12, 2001 .

Done | Local intranet

Suggested Database File Types



- Text
  - Very general, good cross-platform compatibility
  - All processing requires another program
    - Provide sample code for reading in large data sets
- Excel spreadsheet
  - Easier for quick calculations and plotting
  - Needs to be exported for processing by other programs
- HTML files
  - Easy to read on the web
  - Hard to use in other programs
- Applications specific
  - Chemkin input files
  - GT Power models, Matlab/Simulink models, Fluent, etc.

Database Website Functionality

- Search capability
  - Provide on main page
  - Search for keywords in database access page description
  - Output: provide hit-list of links to access pages
- Posting databases
  - User posting ? (probably not)
  - Contact information and procedure for posting by site managers
- Posting of news and comments by users
- User discussion forum?
- Feedback on website

Summary

- Propose a website based aftertreatment database
  - Minor ‘database’ functionality
    - Simple searches
  - Primarily a repository
    - Goal is to make contributions organized and easily accessible
    - Download site
  - Flexible to handle many different types of contributions
- Need contributions
- Very open to feedback and suggestions