Engine Combustion Network

Topic 1: Internal Flow, Near-Nozzle Break-up, Mixing, and Evaporation

Guidance on Experiments and Simulations to be Performed

Sibendu Som: Argonne National Laboratory

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Topics of Interest

Topic 1.1: In-nozzle experiments and simulations

Topic 1.2: Near field spray development and coupled nozzle flow and spray simulations

Topic 1.3: Evaporation and Parametric Variations

Bridging the gap: How spray details (Topic 1) affect Combustion (Topic 2)

Topic 1.1: In-nozzle Experiments and Simulations

David Schmidt: University of Massachusetts
Chris Powell*: Argonne National Laboratory

Experimental Objectives

- Provide boundary conditions for simulations of internal flow
  - Nozzle geometry
  - Rate of injection
  - Needle lift & off-axis motion
- Provide data for validation
  - Radiography at nozzle exit
  - Nozzle flow coefficients
- Assess the uncertainties for all of these parameters

Modeling Objectives

- Define level of confidence of internal flow simulations by validating, where possible, with experimental data
- Quantify internal flow dynamics that are likely to affect spray characteristics of primary atomization
- Assess which physical phenomena are important for including in models
  - Turbulence
  - Compressibility
  - Equilibrium vs. non-equilibrium phase change
  - Dissolved or non-condensable gasses
- Quantities to be compared for validation:
  - Cd, Cv, Ca (for each hole, in the case of spray-B).

Target Injectors

- Spray A
  - Diesel nozzle, single hole, n-dodecane, non-cavitating
  - High resolution (1 mm) X-ray tomography of Nozzle 675
  - Ultra High resolution (0.6 mm) tomography for 678, & 679
  - Lift and wobble measured for all nozzles
  - The target injector will be 675

  http://www.sandia.gov/ecn/cvdata/targetCondition/injectorNozGeom.php
- Spray B
  - Diesel nozzle, 3-hole, n-dodecane, non-cavitating
  - Ultra High resolution (0.6 μm) tomography partially completed
  - Lift and wobble measured for 199, 200 but not yet 201 (use 199 lift and wobble profile for simulations)
  - The target injector will be 201

  http://www.sandia.gov/ecn/cvdata/targetCondition/SpBNozGeo.php

Priority List: Simulations

- Spray A conditions:
  - Injector 675
  - 150 MPa injection pressure vs. time (BoundaryCondition&Data.zip)
  - 100 MPa injection pressure vs. time (BoundaryCondition&Data.zip)
  - Fuel temperature 343 K

- Spray B conditions:
  - Injector 201
  - 150 MPa injection pressure (injection pressure vs. time: Use same as Spray A)
  - 100 MPa (second priority: Use same as Spray A)
  - Fuel temperature 338 K

Data Needed from Experiments

- Dissolved gas content (assume the equilibrium value of 1.28E-3 mole fraction)
- Mass flow rate at the nozzle exit*
  - Spray A target injector
    - Long tube method for ROI
    - Momentum measurements
    - Virtual Injection Rate Generator: http://www.cmt.upv.es/ECN03.aspx
      - Preferred for simulations, data already available
  - Spray B target injector
    - ROI for each hole, individually
    - Virtual Injection Rate Generator: http://www.cmt.upv.es/ECN03.aspx
      - Preferred for simulations, data available end of January
- Needle motion and wobble*
  - Spray A (BoundaryCondition&Data.zip)
  - Spray B (BoundaryCondition&Data.zip)

* These data are provided prior to the simulations being run

Data Needed from Simulations

- Spray A target injector
  - Mass and momentum flow rate and fluctuation distribution at the nozzle exit vs. time
  - Axial slices showing transverse variation of mass flow and momentum at exit for $\theta = 0^{\circ}$. Radial distribution of mass flow and momentum along this axial slice
  - Cd, Cv, Ca

- Spray B target injector
  - Mass and momentum flow rate and fluctuation distribution at the nozzle exit vs. time
  - Axial slices showing transverse variation of mass flow and momentum at exit for $\theta = 0^{\circ}$. Radial distribution of mass flow and momentum along this axial slice
  - Cd, Cv, Ca for each hole
  - Flow split between holes vs. time
  - Vapor fraction at the exit plane as a function of time
  - Iso-surface of 50% vapor by volume

Deadlines

- Experimental data
  - Need ROI (slide 8), geometry (slide 6), and needle motion (slide 8) by January 25
  - Data for validation by March 1
  - Guidelines on how to submit results will be provided shortly
  - Data should be submitted to Chris Powell (cpowell@anl.gov) and cc to Sibendu Som (ssom@anl.gov)

- Computational results:
  - All results must be provided by March 1
  - Guidelines on how to submit results will be provided shortly
  - Data should be submitted to David P. Schmidt (schmidt@ecs.umass.edu) and cc to Sibendu Som (ssom@anl.gov)

Topic 1.2: Near field spray development and coupled nozzle flow and spray simulations

Alan Kastengren*: Argonne National Laboratory
Qingluan Xue: Argonne National Laboratory
Julien Manin: Sandia National Laboratory
Chawki Habchi: IFPEN

Objectives

- Focus on the near nozzle region within first 10 mm
- Obtain quantitative (fuel concentration, droplet size, etc.) and qualitative (macroscopic parameters, optical/x-ray relationship, etc.) information about the breakup process of sprays
- Provide high-fidelity measurements of liquid penetration, liquid mass distribution, and droplet size in the nozzle near field
- Facilitate dynamic coupling of in-nozzle flow and external spray approaches
- Compare the different coupling approaches of in-nozzle flow and external spray
- Encourage high-fidelity simulations near nozzle sprays and liquid jet atomization
- Study the capability of the different modeling approaches (Lagrangian-Eulerian, Eulerian-Eulerian) and CFD frameworks (RANS, LES, DNS) for the simulation of the primary atomization and the cavitation

Anticipated Experimental Results

- Imaging of internal nozzle gas flow and near-nozzle dribble with x-ray phase-contrast imaging
- Microscopic measurements of the initial penetration and spreading angle
- Break up and mixing of the sprays at the end of injection at the microscopic level
- USAXS droplet sizing and perhaps optically measured droplet size as well
- X-ray radiography of Spray B: nozzles 199 and 201
- Ballistic imaging of near-nozzle region

Priority List – Spray A Simulations

- Spray of interest: injector 675
- Condition # 1: Non-evaporating conditions from x-ray radiography at Argonne
  - Ambient pressure: 2 MPa; Ambient temperature with pure N_2: 303 K
  - Injection pressure: 150 MPa; Fuel injection tip temperature: 343 K
- Condition # 2: Parametric variation on Condition #1
  - Ambient pressure: 2 MPa; Ambient temperature with pure N_2: 303 K
  - Injection pressure: 100 MPa; Fuel injection tip temperature: 343 K

Priority List – Spray B Simulations

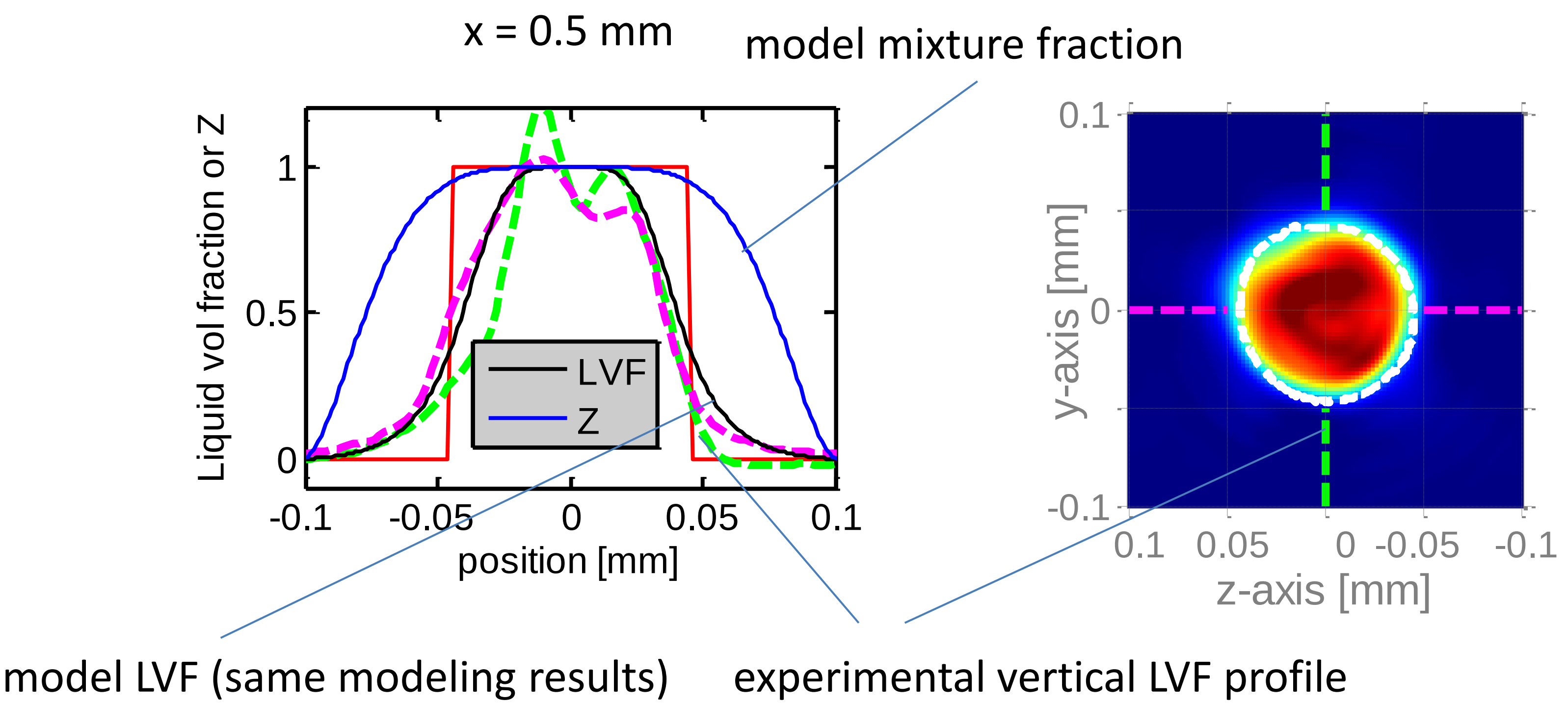
- Spray of interest: Injector 201, plume #3
- Condition # 1, non-evaporating conditions from x-ray measurement at ANL
  - Ambient pressure: 2.01 MPa; Ambient temperature with pure N2: 306 K
  - Injection pressure: 155 MPa; Fuel injection tip temperature: 338 K
- Condition # 2, non-evaporating conditions from x-ray measurement at ANL
  - Ambient pressure: 2 MPa; Ambient temperature with N2: 306 K
  - Injection pressure: 100 MPa; Fuel injection temperature: 338 K

Data Needed from Experiments

- Data needed for initializing Spray A and Spray B simulations are already highlighted in Topic 1.1
- For both injectors: (Data available: BoundaryCondition&Data.zip)
  - Mass flow rate at the nozzle exit from virtual ROI tool from CMT and measured nozzle coefficients
  - Fuel spray penetration vs. time from long-distance microscopy and diffused back-illumination
  - Contour plots of projected liquid density at 0.1 ms and 0.5 ms from Argonne
  - Transverse mass distribution (projected density across the spray) profiles averaged between 0.5 – 1.0 ms:
    - x = 0.1, 0.6, 2, 6, and 10 mm downstream to nozzle exit
    - Projection plane is 0° plane (i.e., plane containing fuel inlet, or projection along the z-axis with the injector in the theta = 0 position)
  - Transverse integrated mass (TIM) vs. axial distance in the near nozzle region @ 0.5 ms
- For Spray A:
  - Liquid volume fraction across cross-section at x = 0.1, 0.6, 2, 6, 10 mm
  - the y-axis cut plane (check slide 17)

Near-nozzle comparisons

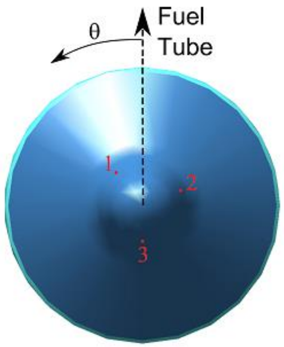
- Much different results if comparing mixture fraction or liquid volume fraction.
- LVF or mixture fraction data derived from x-ray measurements (see SAE 2014-01-1412) compared to a model:



Data Needed from Spray A Simulations

- Mass flow rate at the nozzle exit
- Fuel spray penetration vs. time (0.1% liquid mass fraction)
- Contour plots of projected density in the 0° plane at 0.1 and 0.5 ms after actual SOI
- Projected fuel mass/density (ug/mm^2) profiles across nozzle axis at 0.5 ms after SOI
  - x = 0.1, 0.6, 2, 6, and 10 mm downstream to nozzle exit
  - @ x= 0.6 and 6 mm, @ 0.75 ms and 1 ms after SOI
- 2D contours of liquid volume fraction at x = 0.1, 0.6, 2, 6, 10 mm
- Transverse integrated mass profiles at 0.5 ms after SOI:
  - x = 0.1 mm, 0.6 mm, 2 mm, 6 mm, and 10 mm
- Mean droplet size (SMD) at x = 1, 4, 8 mm at 0.5 ms after SOI
  - Mean SMD at the above axial positions vs. axial position
  - Distributions of SMD vs. radial position at the above axial positions
- Dynamics: peak projected density and Full Width Half Maximum (FWHM) of distribution at x = 0.1, 2, 6 mm from nozzle for entire duration of the injection event (in intervals of 20 µs)

Data Needed from Spray B Simulations



- Spray B target injector (201):
  - Compare results between different plumes for condition # 1
    - Penetration vs. time
    - Transverse mass distribution at 0.1 mm, 2 mm, and 6 mm
    - Mean SMD at 1, 4 mm at 0.5 ms after SOI vs. axial position
- For plume # 3 which is measured at Argonne
  - Contour plots of projected density in the 0° plane at 0.1 and 0.5 ms after actual SOI
  - Projected fuel mass/density (ug/mm^2) profiles across nozzle axis at 0.5 ms after SOI
    - x = 0.1, 0.6, 2, 6, and 10 mm downstream to nozzle exit
    - @ x= 0.6 and 6 mm, @ 0.75 ms and 1 ms after SOI
- 2D contours of liquid volume fraction at x = 0.1, 0.6, 2, 6, 10 mm
- Transverse integrated mass profiles at 0.5 ms after SOI:
  - x = 0.1 mm, 0.6 mm, 2 mm, 6 mm, and 10 mm
- Mean droplet size (SMD) at x = 1, 4, 8 mm at 0.5 ms after SOI
  - Mean SMD at the above axial positions vs. axial position
  - Distributions of SMD vs. radial position at the above axial positions

Deadlines

- Computational results:
  - January 25, 2014: model input data provided
  - February 15, 2014: contact organizers to arrange data format for submission
  - March 1, 2014: all results must be submitted
  - Results should be submitted to:
    - Alan Kastengren (akastengren@anl.gov)
    - Julien Manin (jmanin@sandia.gov)
    - Qingluan Xue (qxue@anl.gov)
    - Chawki Habchi (chawki.habchi@ifpen.fr)
    - Sibendu Som (ssom@anl.gov)

Engine Combustion Network

Topic 1.3: Evaporation and Parametric Variations

Alessandro Montanaro: – CNR Instituto Motori
Tommaso Lucchini*: – Politecnico di Milano

Global Objectives

- Focus on non-combusting conditions
- Understanding how the spray development in the far field is influenced by variation of operating conditions :
  - Injection pressure
  - Ambient density
  - Ambient temperature
  - Nozzle geometry
- How different experimental techniques affect measurements?
- Are multi-dimensional models capable to reproduce experimental trends?

Objectives

Experimental:

- Define a set of operating conditions to build a database of experiments for Spray-B configuration.
- Understanding how results are repeatable in different institutions (Spray A and Spray B).
- Understanding influence of different nozzle serial numbers on spray evolution (Spray A and Spray B).

Simulation:

- How different models reproduce the effects of different operating conditions on spray evolution?
- To compare different approaches (Eulerian-Lagrangian, Eulerian-Eulerian, …) and, within the same approach, different sub-models.
- Understanding how spray evolution from multi-hole nozzle is affected by mesh structure.

Required Experimental data for Spray-A

Priority list : experimental conditions to be tested

Priority level	T [K]	density [kg/m^3]	Pressure [MPa]	Fuel	T fuel [K]	Injection duration [ms]
1	900	22.8	150	n-dodecane	363	≥1.5
2	900	22.8	100	n-dodecane	363	≥1.5
3	900	22.8	50	n-dodecane	363	≥1.5
4	900	7.6	150	n-dodecane	363	≥1.5
5	900	15.2	150	n-dodecane	363	≥1.5
6	700	22.8	150	n-dodecane	363	≥1.5
7	1000	22.8	150	n-dodecane	363	≥1.5
8	1100	22.8	150	n-dodecane	363	≥1.5
9	700	22.8	50	n-dodecane	363	≥1.5
10	440	22.8	150	n-dodecane	363	≥1.5
11	303	22.8	150	n-dodecane	363	≥1.5

Required Experimental data for Spray-A

Experimental data to be provided

- Injected fuel mass flow rate
- Liquid spray penetration versus time
- Liquid spray penetration (steady)
- Vapor penetration versus time
- Radial distribution of mixture fraction and variance at 25 and 45 mm from injector at 1.5 ms after SOI.
- Axial distribution of mixture fraction and variance at 1.5 ms after SOI.
- Radial distribution of axial and radial velocity components at 25 and 45 mm from injector at 1.5 ms after SOI
- Axial velocity distribution at 1.5 ms after SOI.

Additional information (only if it is different from Spray A)

- Details about the used test-rig.
- Details about vessel temperature distribution at start of injection.
- Details about techniques used for experiments.

Information for Setting-up Spray A simulations

- Ambient conditions: use SANDIA ECN experimental data search utility.
- Injected mass flow rate profile: use CMT mass flow rate generator.
- Nozzle geometry: use 675 dimensions
- Tune the model on baseline Spray A condition (priority 1) with 1.5 ms injection duration.

Required Data from Spray A simulations

Simulated operating points: same of experiments

Simulated data to be provided

- Liquid spray penetration versus time
- Liquid spray penetration (steady)
- Vapor penetration versus time
- Radial distribution of mixture fraction and variance at 0.1, 0.6, 2, 5, 6, 10, 25, and 45 mm from injector at 1.5 ms after SOI
  - Vapor-phase and total (liquid and vapor) mixture fraction.
  - For only priority 1, 6, 10 (in slide 24)
- Axial distribution of mixture fraction and variance along the centerline at 1.5 ms after SOI.
- Radial distribution of axial and radial velocity components at 0.6, 5, 10, 25 and 45 mm from injector at 1.5 ms after SOI
  - For only priority 1, 6, 10 (in slide 24)
- Axial velocity distribution at 1.5 ms after SOI.

Experimental Data Requested for Spray-B*

Priority level	T [K]	density [kg/m^3]	Pressure [MPa]	Fuel	T fuel [K]	Injection duration [ms]
1	900	22.8	150	n-dodecane	363	1.5
2	440	22.8	150	n-dodecane	363	1.5
3	303	22.8	150	n-dodecane	363	1.5
4	1100	22.8	150	n-dodecane	363	1.5

* It is understood that all the above Spray B data may not be available by March 1st, hence please plan your experiments as per the noted priority

Experimental data to be provided

- Injected fuel mass flow rate: available from the virtual rate generator at CMT
- Liquid spray penetration versus time
- Liquid spray penetration (steady)
- Vapor penetration versus time

Additional information

- Details about the used test-rig
- Details about vessel temperature distribution at start of injection
- Details about techniques used for experiments

Information for Setting-up Spray B simulations

- Ambient conditions: use SANDIA ECN experimental data search utility.
- Injected mass flow rate profile: use CMT rate of injection generator
- Nozzle geometry specifications for 201
- Use the same set of model constant that were obtained for Spray A baseline condition

Spray B simulations

Objective: understanding how mesh structure affects spray evolution.

- All three holes must be included in simulations
- Use same spray parameters from spray A model tuning

Simulated operating points

Priority level	T [K]	density [kg/m^3]	Pressure [MPa]	Fuel	T fuel [K]	Injection duration [ms]
1	900	22.8	150	n-dodecane	363	1.5
2	440	22.8	150	n-dodecane	363	1.5

Required Data from Spray B simulations

- Liquid spray penetration versus time for each plume
- Liquid spray penetration (steady) for each plume
- Vapor penetration for each plume
- Projected gas velocity along the axis of each plume
- Radial velocity distribution for each plume at 2, 10, and 20 mm axial distance from nozzle
- Radial mixture fraction distribution for each plume at 2, 10, and 20 mm axial distance from nozzle.
- Radial mixture fraction variance distribution for each plume at 2, 10, and 20 mm axial distance from nozzle.

Deadlines

- Computational and experimental results:
  - Contact organizers by February 15th for data submission format
  - All results must be provided by March 1st
  - Experimental results to be sent to Alessandro Montanaro (alemon@im.cnr.it) and cc to Sibendu Som (ssom@anl.gov)
  - Simulation results should be sent to Tommaso Lucchini and Roberto Torelli (tommaso.lucchini@polimi.it , roberto.torelli@polimi.it) and and cc to Sibendu Som (ssom@anl.gov)

Bridging the gap: How Spray details (Topic 1) affect Combustion (Topic 2)

Yuanjiang Pei, Sibendu Som: Argonne National Laboratory
Jose Garcia: CMT-Motores Termicos

Objectives

- Designed to bridge-the-gap between spray (Topic 1) and combustion (Topic 2) for Spray A
- How do the differences in boundary conditions and spray characteristics influence combustion characteristics?
- Can simulations using the best boundary conditions available, capture these trends?
- Why differences in spray characteristics do not seem to influence the combustion behavior?
- What are the most sensitive variables for different targets of spray and combustion characteristics? - (Global Sensitivity Analysis)

Boundary Conditions

Facility	Nominal				SNL				CMT			
Combustion vessel	---				constant-volume preburn				constant-pressure flow			
Fuel	n-dodecane											
Injector Number #	---				210677				210675			
Injector diameter [mm]	0.090				0.0837				0.0894			
Discharge coefficient	0.86				0.89				0.9			
ROI	ECN2 recommended ROI_NOM.txt				SNL ROI_SNL.txt				CMT ROI_CMT.txt			
Reacting	No	Yes			No	Yes			No	Yes		
Ambient temperature [K]	900	800	900	1100	891.9	800.8	902	1112.3	896	810.8	899.9	1100
Injection pressure [MPa]	150	150	150	150	152.7	154.8	152.8	152.6	150	150	150	150
Injection duration [ms]	1.54	6.1	6.1	6.1	1.54	6.1	6.1	6.1	1.54	6.1	6.1	6.1
Mass injected [mg]	3.46	14	14	14	3.46	14	14	14	3.46	14	14	14
Ambient density [Kg/m^3]	22.8	22.8	22.8	22.8	23.01	22.76	22.81	22.7	22.8	22.5	22.8	22.8
Initial mole composition [%]	O_2=0; N_2=89.71; CO_2=6.52; H_2O=3.77	O_2=15; N_2=75.15; CO_2=6.22; H_2O=3.62			O_2=0; N_2=89.71; CO_2=6.52; H_2O=3.77	O_2=15; N_2=75.15; CO_2=6.22; H_2O=3.62			O_2=0; N_2=100	O_2=15.01 ; N_2=85	O_2=15.1, N_2=84.9	O_2=15.1, N_2=84.9
						OH [ppb]						
						4	7.8	168				
Fuel temperature [K]	363	363	363	363	373	373	373	373	386	384	386	386
Ambient pressure (MPa)	6.05	5.25	5.94	7.3	6.05	5.25	5.94	7.3	6	5.4	6.09	7.3

- **For injection parameters, one can choose injection pressure or mass injected and injection duration, you may choose the one that suits your need.**
- **OH mole fraction is obtained from *Nesbitt et al. 2011*, approximations are made.**

Guidelines for Simulations (Spray A)

- **Run 3 simulations with nominal, SNL and CMT on each conditions listed below, and use the available boundary conditions (cf. Slide 3) to capture the variation of the experiments.**
    - One non-reacting case at 900 K
    - Three ambient T conditions for reacting cases, 800 K, 900 K and 1100 K.
- **Submit the following results using recommended definitions by each topic organizer:**
    - Global Sauter mean diameter vs. time
    - Liquid length vs. time
    - Vapor penetration length vs. time
    - Lift-off length vs. time
    - Ignition delay
    - Modeling and numerical details provided to each topic organizer i.e., Sibendu Som and Jose Garcia
    - Please report the boundary conditions you used that are different than the ones listed in the table of last slide in any case.
- **Additional data may be requested based on analysis to gain further insight**

Data submission deadline

- Submission deadline: March 1st 2014
- Please send the data to Yuanjiang Pei (ypei@anl.gov)
- Format for the data submission (both line and contour plots) will be made available soon