

## Framework Document for the CMFR Workshop June 6-7, 2006

The goal of the Collaboratory for Multiphase Flow Research (CMFR) workshop is to ensure that by 2015 multiphase science based computer simulations play a significant role in the design, operation, and troubleshooting of multiphase flow devices in fossil fuel processing plants (e.g., CCPI and/or FutureGen). The organizational structure of the CMFR workshop is based on four technical tracks which align themselves with DOE/NETL's technology roadmap (see Figure 1) for future power plants. Within each technical track the CMFR workshop objectives are focused on how computational multiphase flow research can impact key barrier issues in the technology development of future power plants.

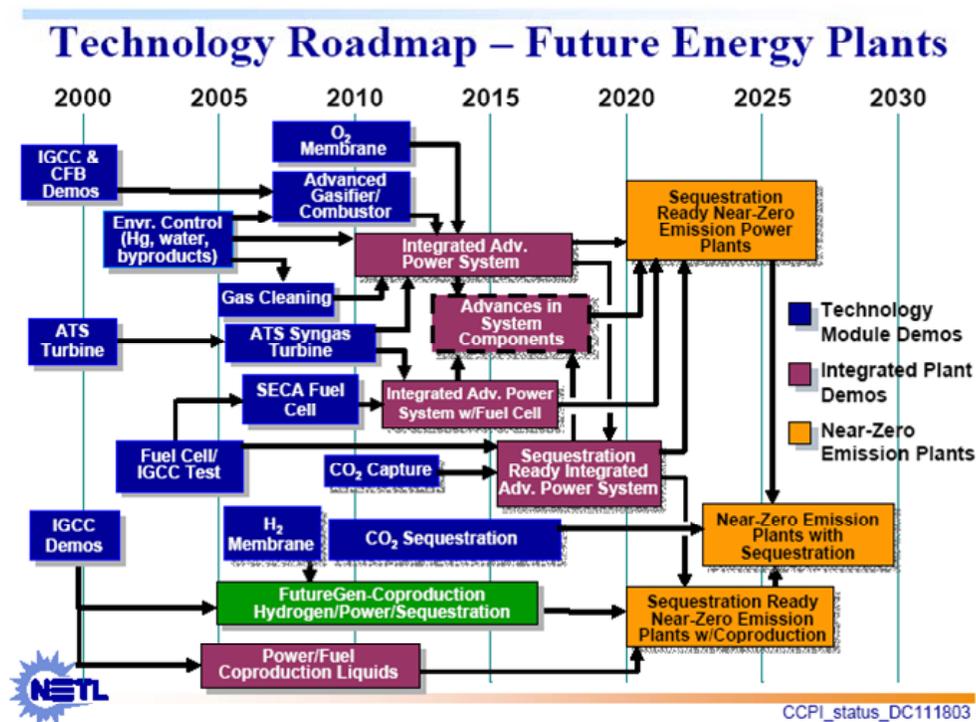


Figure 1 Technology Roadmap – Future Energy Plants

The following table shows the relation of the milestones on the technology roadmap for future energy plants to the technical tracks. The details of the technical tracks are given in the appendix. The energy technology and barrier issues relevant to each technical track are given there. The research topics are also applicable to other NETL technologies and to a broad range of chemical, petroleum and pharmaceutical processes.

Technical Track	Relation to Future Energy Plants Technology Roadmap
1. Dense Gas-Solids and Granular Flows	IGCC & CFB, Advanced gasifier/combustor, Gas Cleaning
2. Dilute Gas-Solids Flows	IGCC & CFB, Advanced gasifier/combustor, Gas Cleaning
3. Liquid-solids/Gas-liquid flows	Gas cleaning, Fuel Cell, CO <sub>2</sub> capture, CO <sub>2</sub> sequestration, FutureGen-Coproduction, Coproduction of Liquid fuels
4. Computational Physics and Applications	This track deals with the development and application of physics-based computational models to the technologies listed under Tracks 1-3.

## Appendix: Technical Tracks

<b>Track 1</b>		<b>Dense Gas-Solids Flows and Granular Flows</b>			
Chair	Paul Mort (P&G)	CoChair	J. McCarthy (U. Pittsburgh)	NETL	Ron Breault
Members					
Technology and Barrier Issues	<b>Energy:</b> Gasifiers, chemical looping process, standpipe, coal storage, transport and feeding, CO <sub>2</sub> capture and sequestration, hot-gas cleanup, co-feeding coal with alternative feedstock, Shale oil extraction, Oxy-coal combustion, oxygen-free gasification, direct reduction of iron ore				
	<b>Others:</b> FCC stripper and regenerator, particle coating				
Discussion Topics	<ul style="list-style-type: none"> <li>• What are the modeling approaches? What can be modeled with confidence? How well are the models validated? What well defined experiments exist? What other experiments are needed? What information does the design engineers need? What short and long term advances are needed in the models?</li> <li>• Research Topics               <ul style="list-style-type: none"> <li>○ Particle size, shape and their distribution</li> <li>○ moisture content and structural stability</li> <li>○ Yield, arching, shear bands, clogging, vibration</li> <li>○ Cohesive inter-particle forces</li> <li>○ Frictional contact between particles</li> <li>○ Kinetic theory, frictional theory</li> <li>○ Adsorption/Desorption</li> <li>○ segregation or mixing of particles of different size and density</li> <li>○ Interphase Heat and mass transfer</li> <li>○ Chemical reactions</li> <li>○ Transition to dilute flow</li> </ul> </li> </ul>				

<b>Track 2</b>		<b>Dilute Gas-Solids Flows</b>			
Chair	R. Patel (Exxon-Mobil)	CoChair	S. Subramaniam (Iowa State U.)	NETL	Sofiane Benyahia
Members					
Technology and Barrier Issues	<b>Energy:</b> Pulverized coal combustion, pneumatic conveying, transport and deposition of ash/slag, particle separation devices, biomass cofiring, transport desulfurizer, transport gasifier				
	<b>Others:</b> FCC riser,				
Discussion Topics	<ul style="list-style-type: none"> <li>• What are the modeling approaches? What can be modeled with confidence? How well are the models validated? What well defined experiments exist? What other experiments are needed? What information does the design engineers need? What short and long term advances are needed in the models?</li> </ul>				

	<ul style="list-style-type: none"> <li>• Research Topics <ul style="list-style-type: none"> <li>○ Fluid-particle interaction</li> <li>○ Particle-particle interactions</li> <li>○ Extending single-phase LES or DNS to include particles</li> <li>○ Turbulence and transition to turbulence modified by particles</li> <li>○ Turbulent dispersion and its effects on chemical reaction rate</li> <li>○ Chemical reactions</li> <li>○ Radiation</li> <li>○ Interphase heat and mass transfer</li> <li>○ Transition to dense flow</li> </ul> </li> </ul>
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Track 3		Liquid-solids/Gas-liquid flows			
Chair	P. Ma (Air Products)	CoChair	R. Fox (Iowa State U.)	NETL	Isaac Gamwo
Members					
Technology and Barrier Issues	<p><b>Energy:</b> Fischer-Tropsch reactor, coal-slurry feeder, slurry bubble column reactors, hydrocyclones, trickle bed reactors, Absorbers, scrubber, CO<sub>2</sub> capture and sequestration, fuel cell, bubble column reactors, air-lift reactor</p> <p><b>Others:</b></p>				
Discussion Topics	<ul style="list-style-type: none"> <li>• What are the modeling approaches? What can be modeled with confidence? How well are the models validated? What well defined experiments exist? What other experiments are needed? What information does the design engineers need? What short and long term advances are needed in the models?</li> <li>• Research Topics <ul style="list-style-type: none"> <li>○ Absorption/Desorption</li> <li>○ Rate of droplets entrainment to walls</li> <li>○ Effect of wall heat flux on deposition of droplets</li> <li>○ slug formation and flow transition from disperse to slugging</li> <li>○ Phase distribution in bubbly flows</li> <li>○ topological changes at relatively sharp spatial regions</li> <li>○ Interface drag and other forces such as lift force, added mass...</li> <li>○ Prediction of regime transition: discrete bubble flow, dispersed bubble flow, coalesced bubble flow, slug flow, churn flow, bridging flow and annular flow.</li> <li>○ Chemical reactions</li> </ul> </li> </ul>				

Track 4		Computational Physics and Applications			
Chair	Ray Cocco (Dow)	CoChair	C. Hrenya (U. Colorado)	NETL	Chris Guenther
Members					
Technology	Common for all technologies				

and Barrier Issues	
Discussion Topics	<ul style="list-style-type: none"><li>• How to best exploit the enormous amount of data generated by simulations?</li><li>• Research Topics<ul style="list-style-type: none"><li>○ Numerical techniques</li><li>○ Eulerian-Eulerian, DEM, LBM, VOF</li><li>○ Computational speed in transient calculations</li><li>○ Parallelization</li><li>○ Verification and Validation</li></ul></li><li>• How to promote the use of computational models by industry?<ul style="list-style-type: none"><li>○ Identifying relevant problems</li><li>○ Outreach activities</li></ul></li></ul>