

The Role of GPU Computing in Accelerating Commercialization and Scale-up of Thermochemical Conversion Processes

Presented by:

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Presented at:

tcbi  **mass**

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Thermochemical Conversion Processes and Fluidized Beds

Many thermochemical conversion processes use fluidized beds

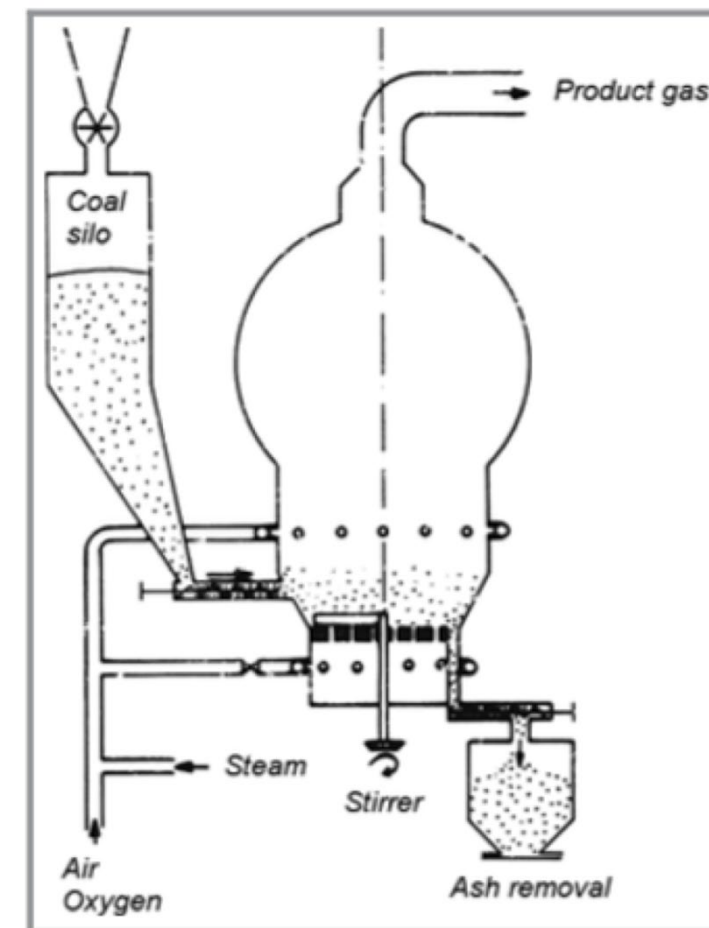
- Fluidized beds, circulating fluidized beds
- Other fluid-particle processes

Benefits of fluidized beds

- Good mixing and heat transfer
- Move particles between units easily
- Handle broad range of particle properties

Complexity

- Hydrodynamics, thermodynamics, chemical reactions
- Varying role of particle phase (heat transfer, reactant, product, sorbent, catalyst, etc.)
- Wide range of length and time scales



Early Winkler Gasifier ~1930s

Fluidized Bed Simulation

Improving performance through simulation

- Determine root cause of phenomena
- Reduce risk of changes through virtual testing
- Identify additional optimization opportunities
- Accelerated R&D, commercialization and scale-up

Simulation results in this presentation created using Barracuda Virtual Reactor

- Hydrodynamics, thermal, chemical reactions in industrial units
- Parallelized using GPU and multi-GPU acceleration



CPU and GPU Parallelization

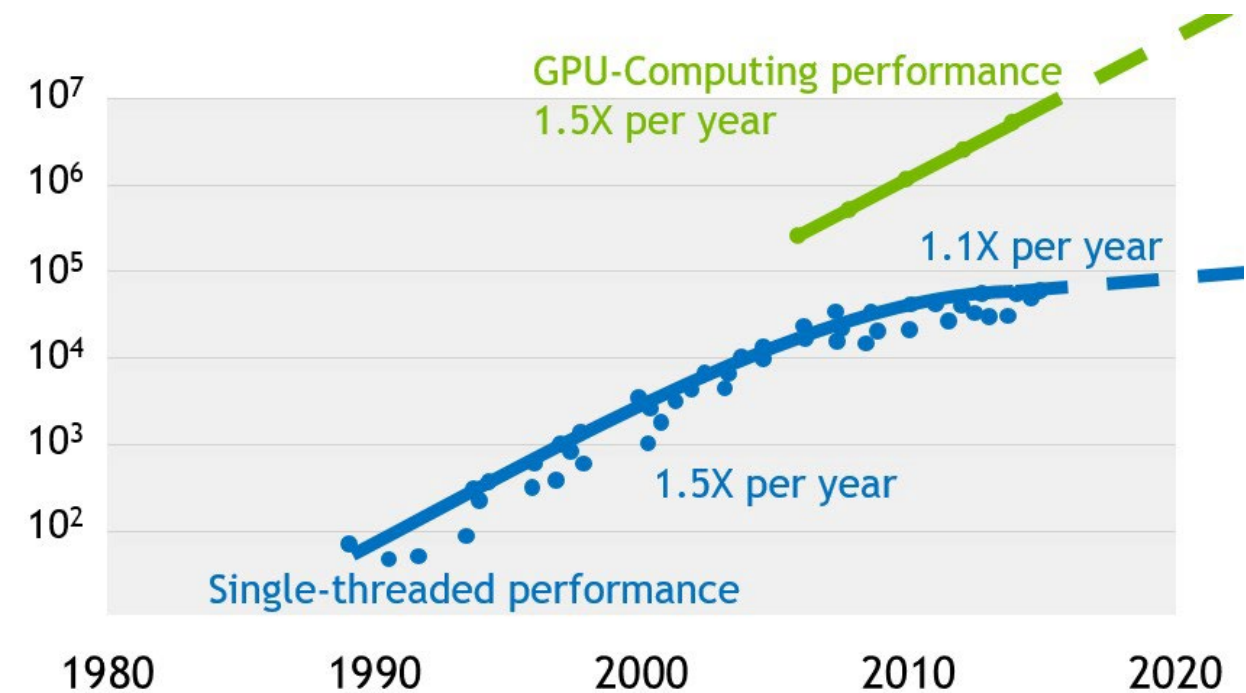
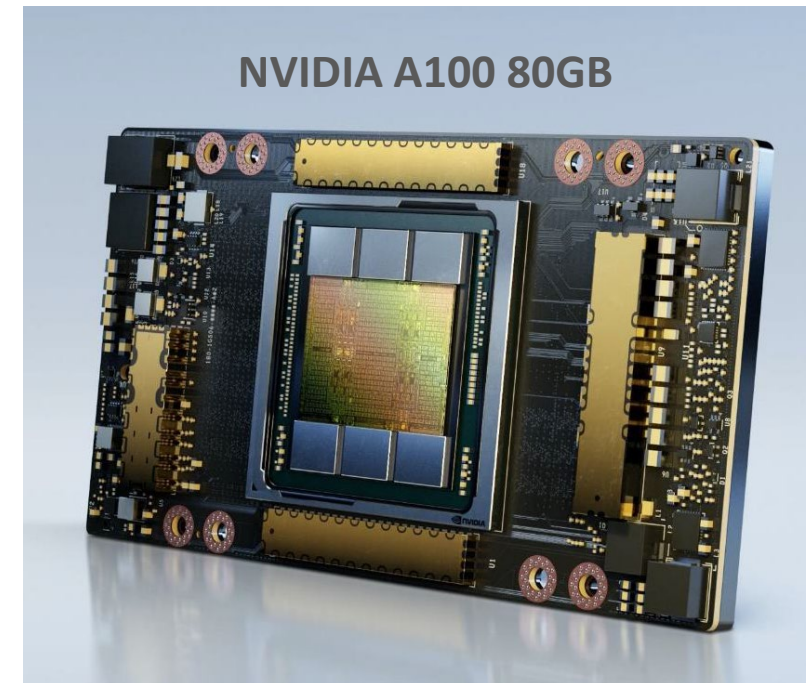
CPU parallelization

- Multiple CPUs solving the same system
- CPU speed doubled every 1.5 – 2 years
- Thermal limitations, trend toward increasing core counts (~2010)

GPU parallelization

- Computer graphics (late 1990s)
- Scientific computing (2000s)
- Today GPU core counts ~8,000 vs 24-96 in most powerful CPUs

Significant differences observed in recent years



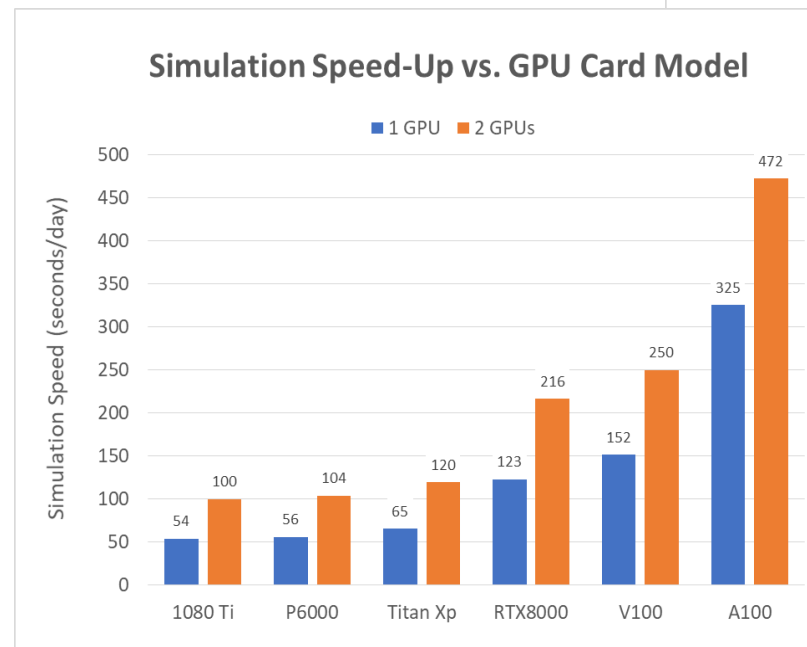
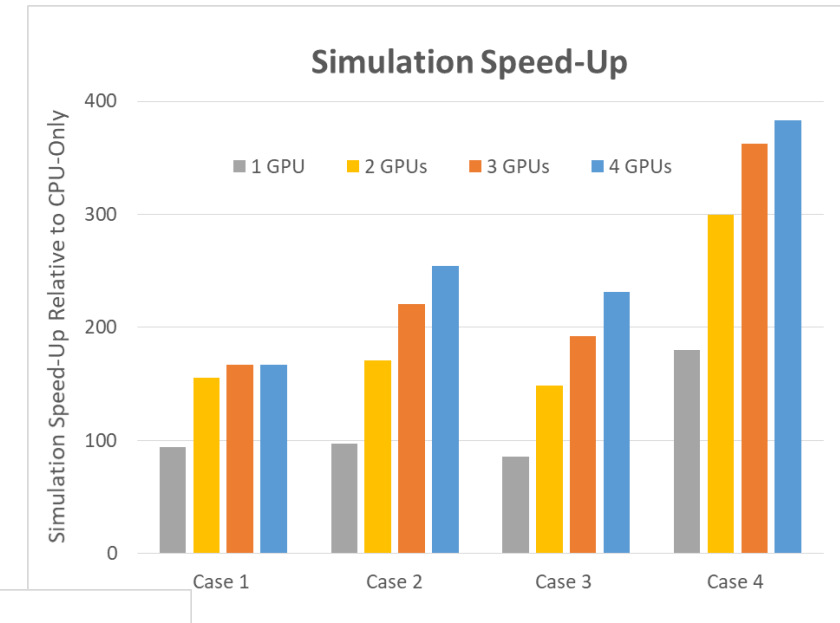
GPU Speed-Up of Fluidized Bed Simulations

GPU parallelization of fluidized bed simulations

- Single GPU parallel (2013-2014)
- Multi-GPU parallel (2021)
- Currently seeing 50x – 400x speed-up over serial

Sources of speed up

- GPU porting of most compute-intensive functions
- Restructuring code for GPU efficiency
- Advances in the NVIDIA software and hardware stack



Why Speed? 1. Faster Results and More Virtual Testing

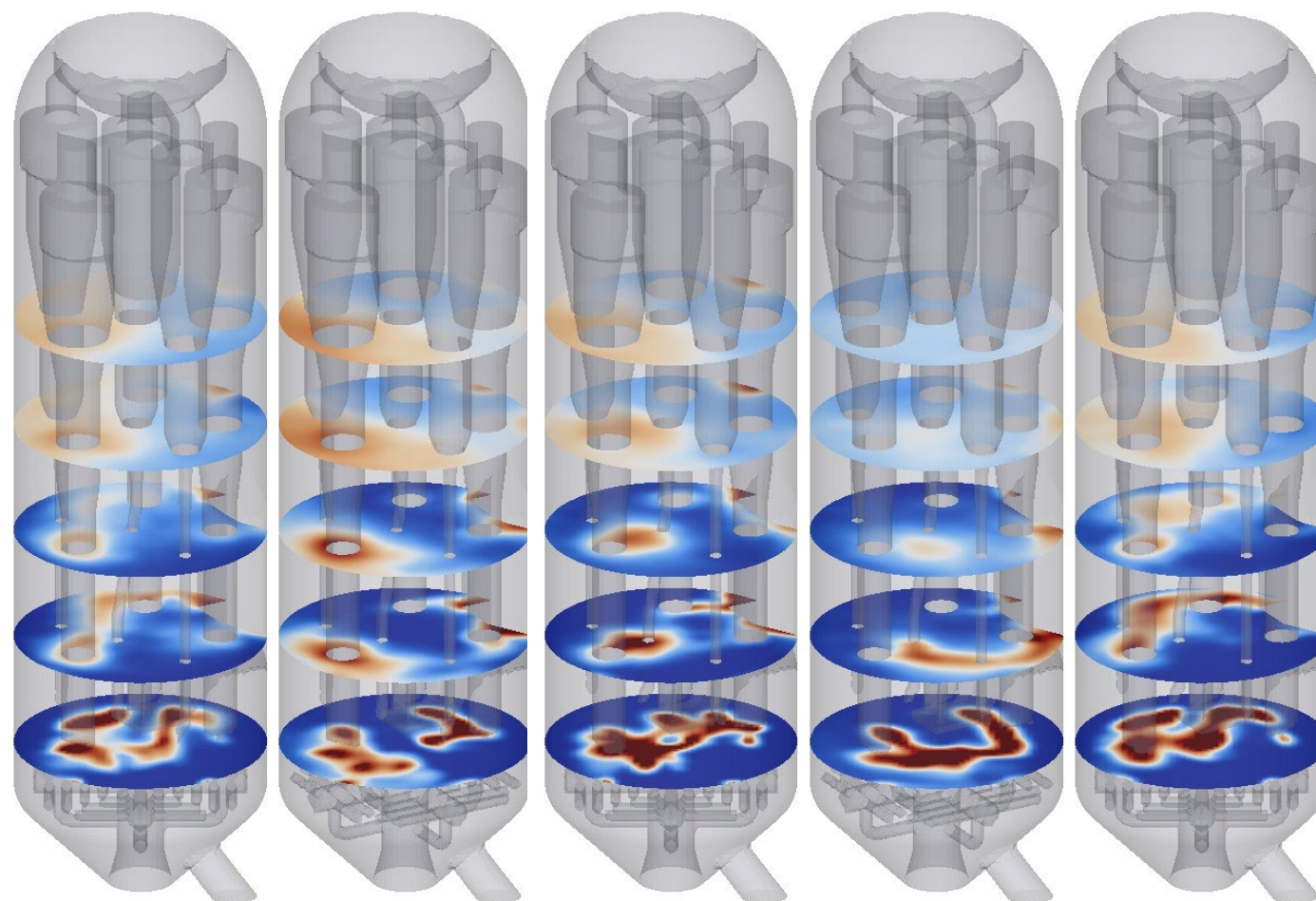
Consider a 150x-200x speed-up:

- Faster: week long simulation in an hour
- More: 150 – 200 simulations in a week

Implications of more virtual testing

- Increase exploration of research space
- Fewer physical test performed
- Toward enabling AI / ML

New technologies brought to market faster, at lower cost



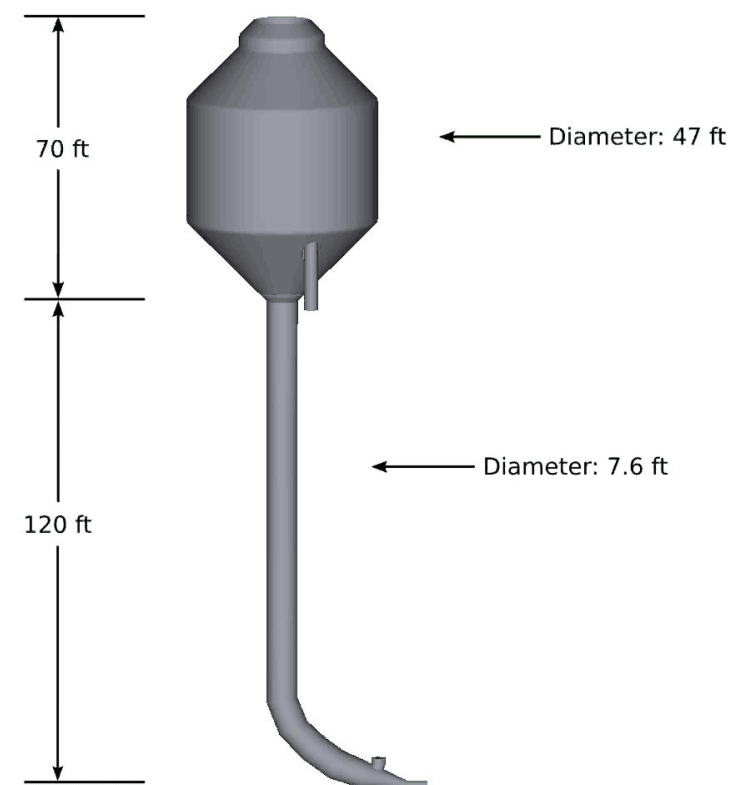
Why Speed? 2. Higher Fidelity Models

Detailed simulation (~2012)

- Subdivided into 3 separate models
- Model 1: 2 days
- Model 2: 3 years
- Model 3: 64 days



Commercial FCC Regenerator Simulation



Combined Geometry: Spent Cat Riser + Regenerator



Why Speed? 2. Higher Fidelity Models

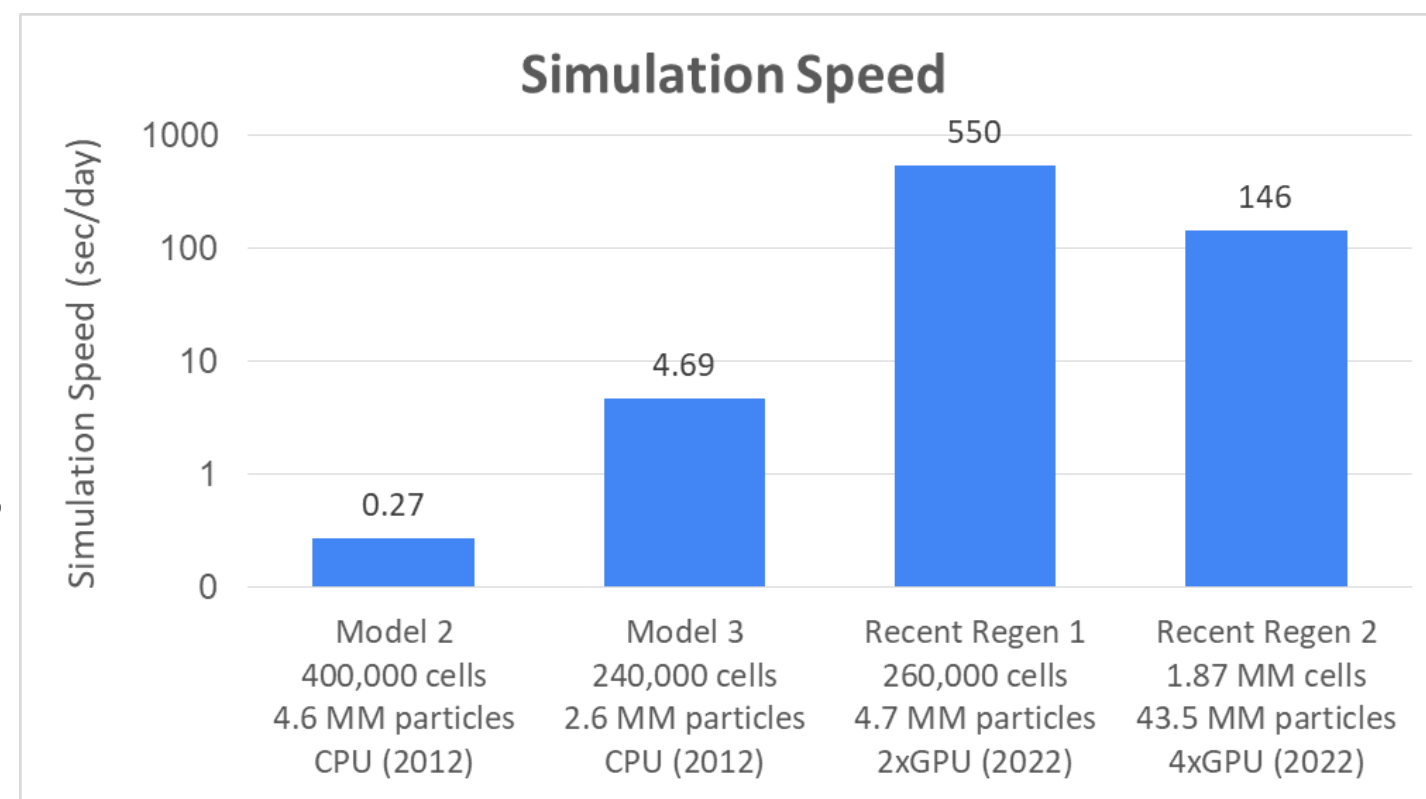
Detailed simulation (~2012)

- Subdivided into 3 separate models
- Model 1: 2 days
- Model 2: 3 years
- Model 3: 64 days

Comparable models now run in 12-48 hours

No modeler would construct the same model today

- Larger model domain
- Finer resolution
- More / detailed physical model
- Complex chemical reaction mechanisms, etc.



Example courtesy of:



Why Speed? 3. Making the Impossible, Possible

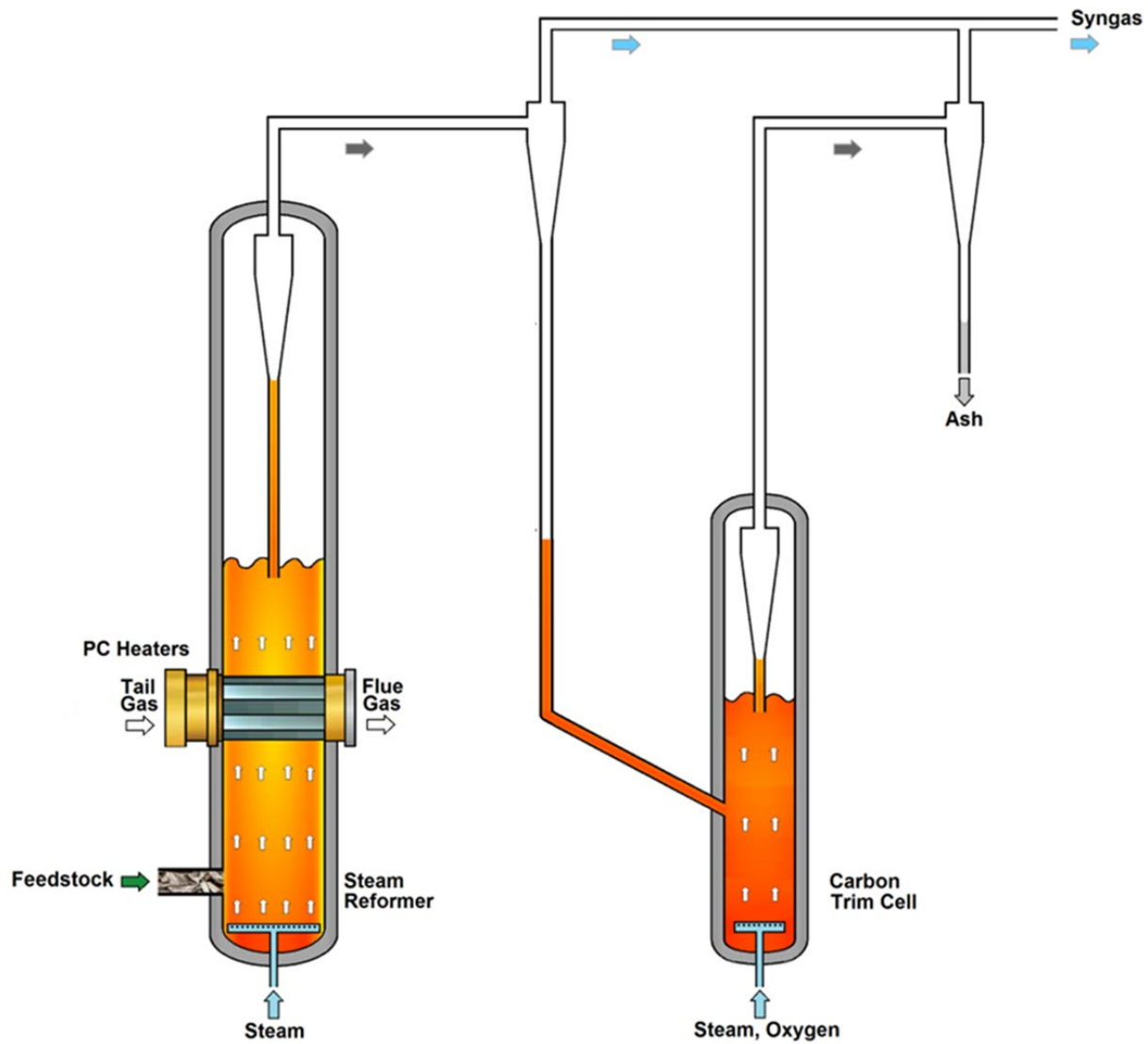
ThermoChem Recovery International (TRI) case study

- Technology enabling biorefineries for green fuels, chemicals and power
- Wide range of feedstocks (biomass, black liquor, MSW)
- High carbon conversion

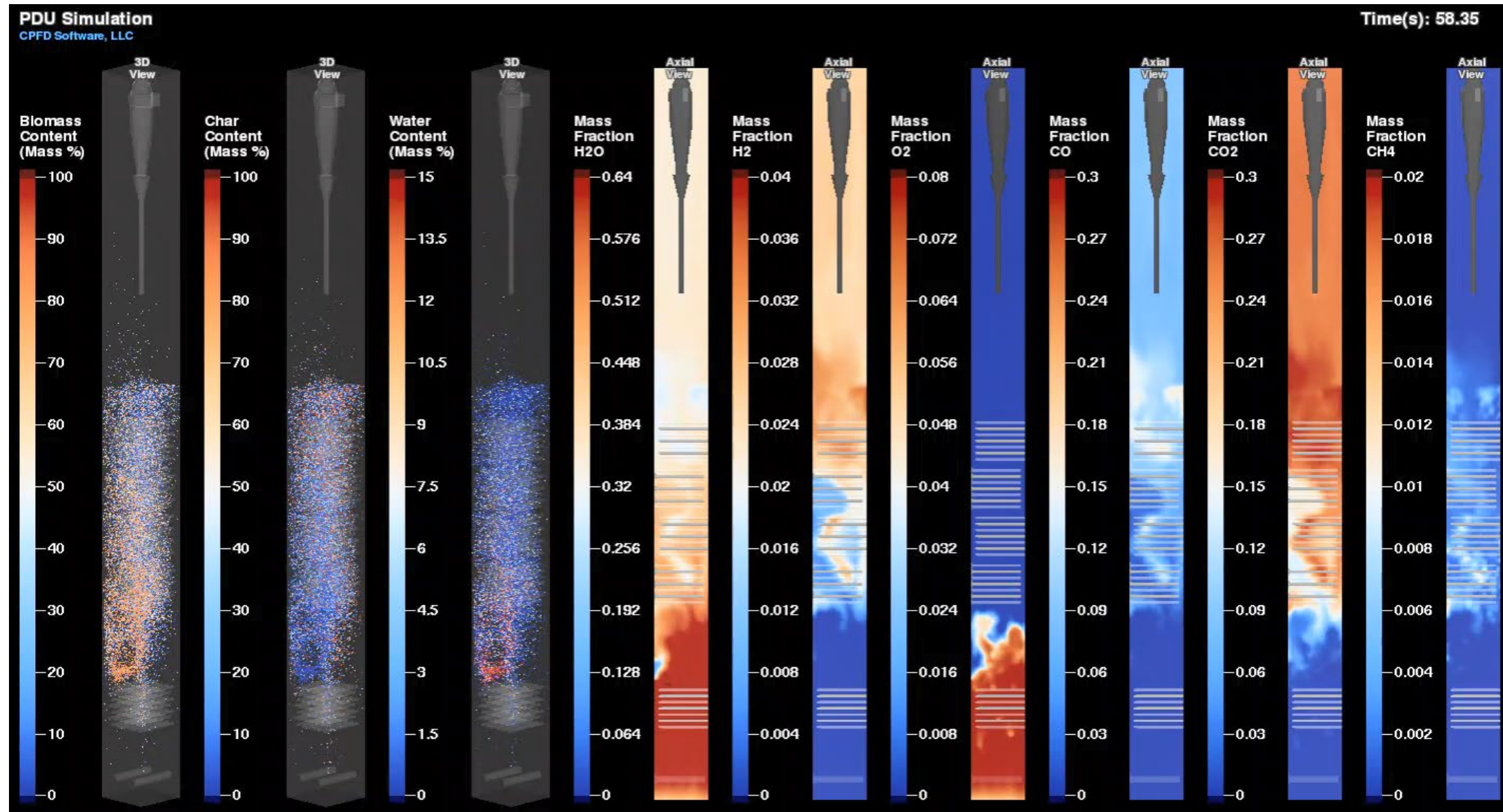
Acceleration of technology development, commercialization and scale-up



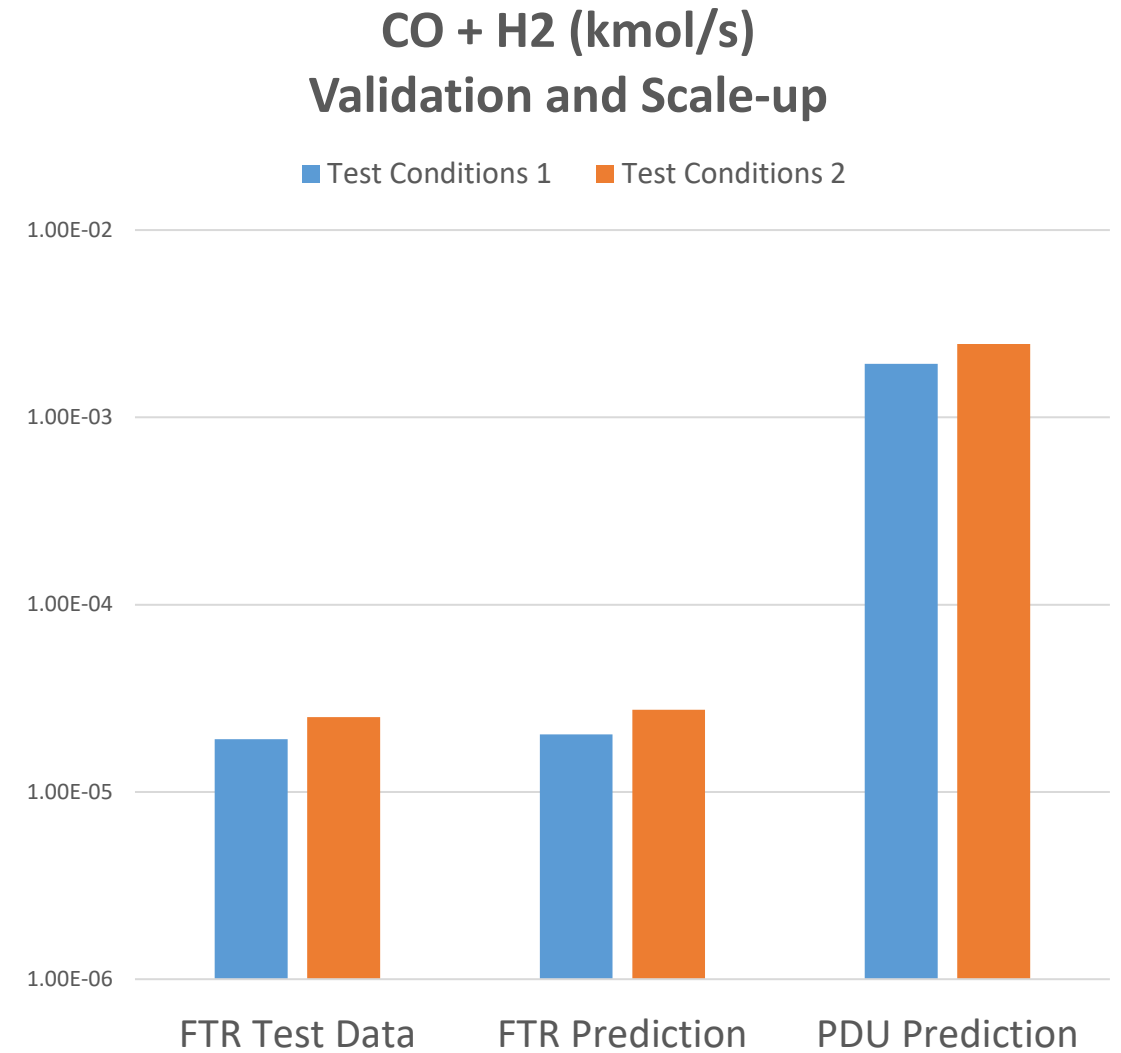
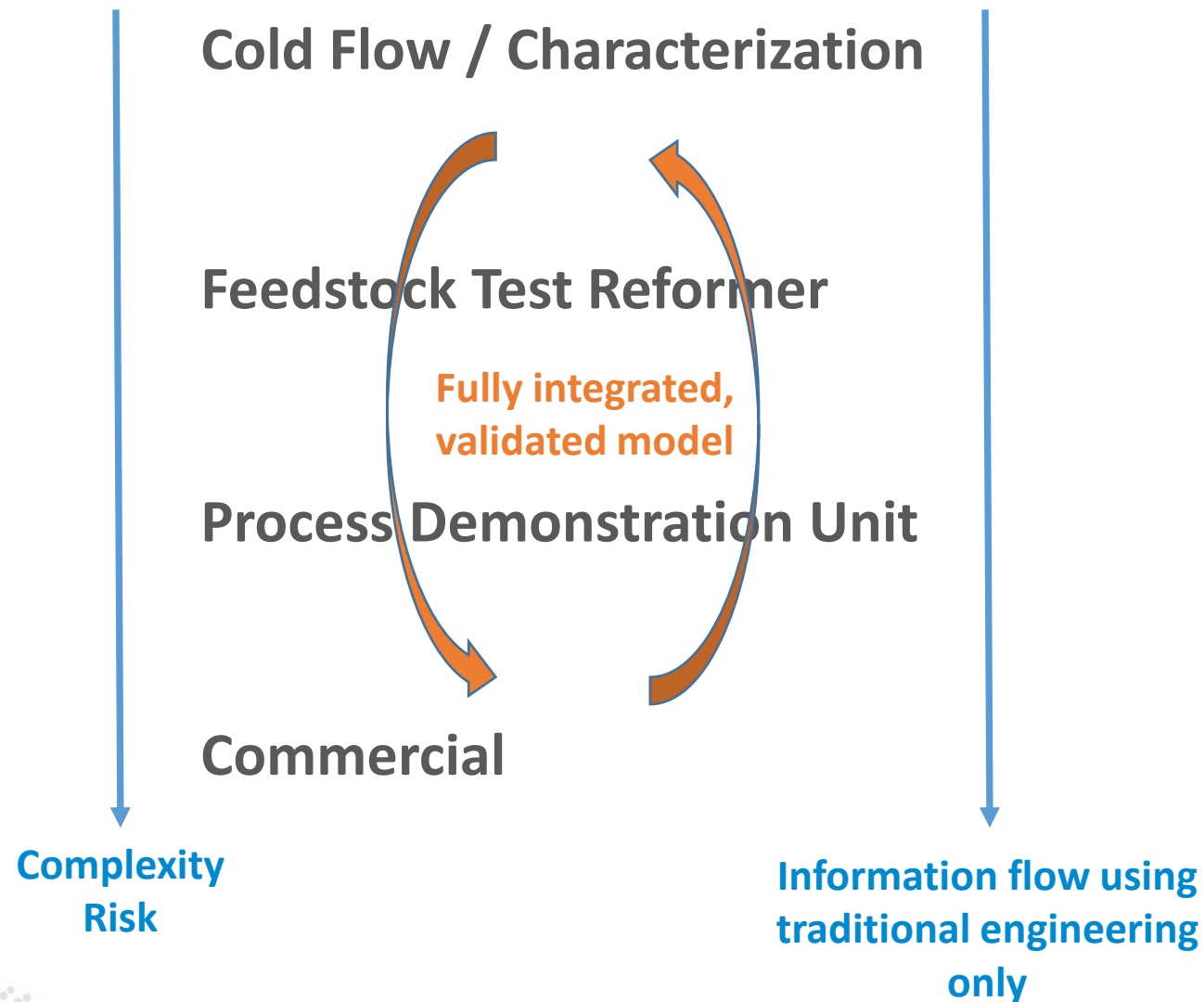
Process, and Process Demonstration Unit (PDU)



TRI PDU Steam Reformer Simulations



Digital Syngas Model used at Every Scale



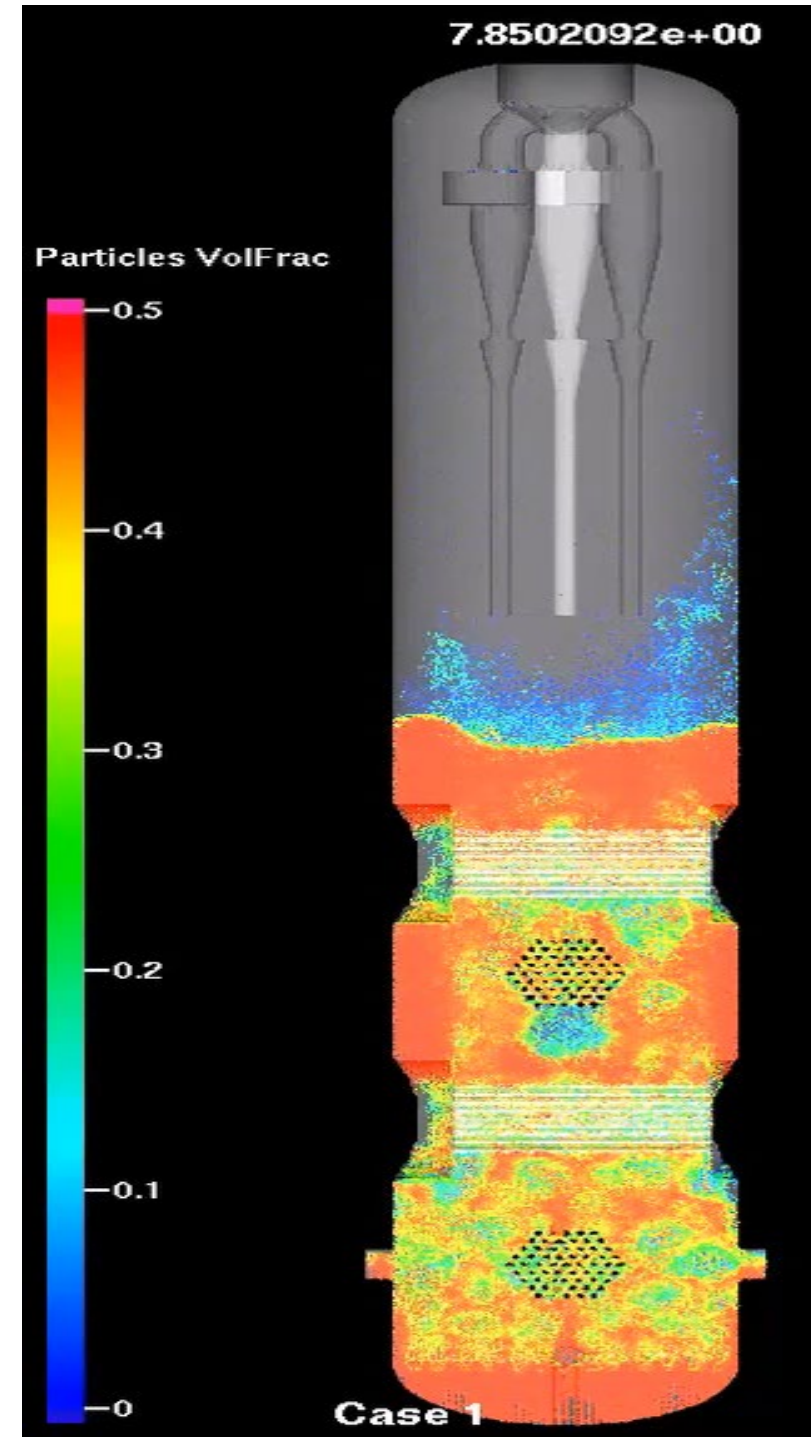
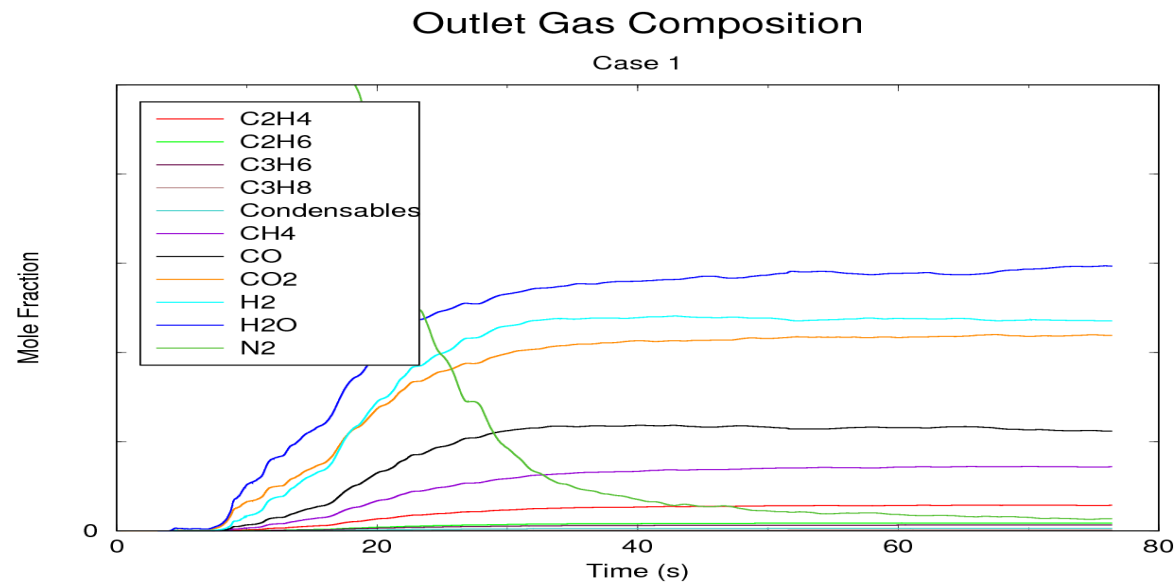
Commercial Simulations

Feedstocks

- Black liquor, forest residuals, MSW

Scales

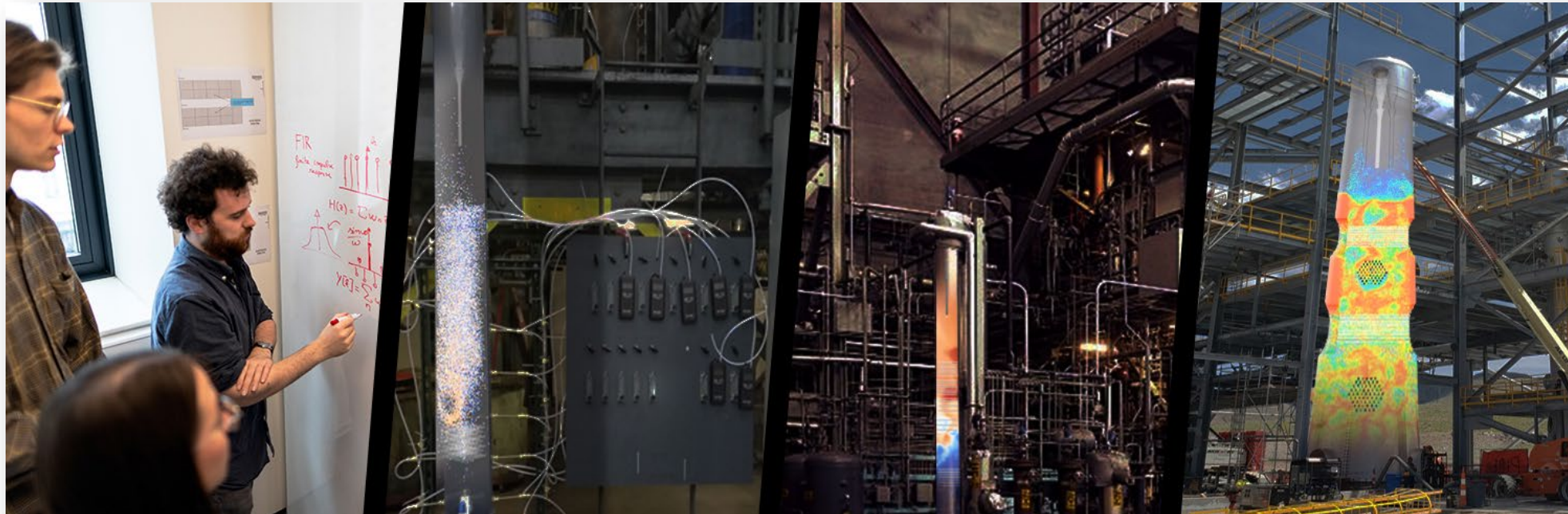
- Recent commercial designs at 500, 1,000 and 2,000 dtpd feedstock throughput



Example courtesy of:



Why Speed? 3. Making the Impossible, Possible



1,500x speed-up since 2009

- Highly Commended by IChemE at 2020 Global Awards for Process Automation and Digitalization

Complexity in today's models was physically impossible to simulate in the past!

Accessibility of GPU Computing Resources

Benefits

- No need for costly CPU cluster
- GPU innovation is ongoing

On-premise GPU resources

- Workstation computers
- Can add or upgrade individual GPUs
- Multi-GPU systems available without customization

Major cloud service providers now offer GPU resources



NVIDIA DGX
Station



Conclusions

GPU computing has transformed what is possible for simulations of fluidized beds which are widely used in thermochemical conversion processes

Impact of GPU and multi-GPU speed-up

- Faster simulation times
- More virtual testing in same time frame
- Higher fidelity models
- Making the impossible, possible

GPU technology is continuing to innovate and broadly accessible today

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