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National Aeronautics and Space Administration

COMSOL Grab Bag

How to use a versatile CFD code to solve interesting problems from cryogenic storage to biofuel production

Dr. Emily Nelson

The benefits of computational methods

CFD permits us to see the unviewable

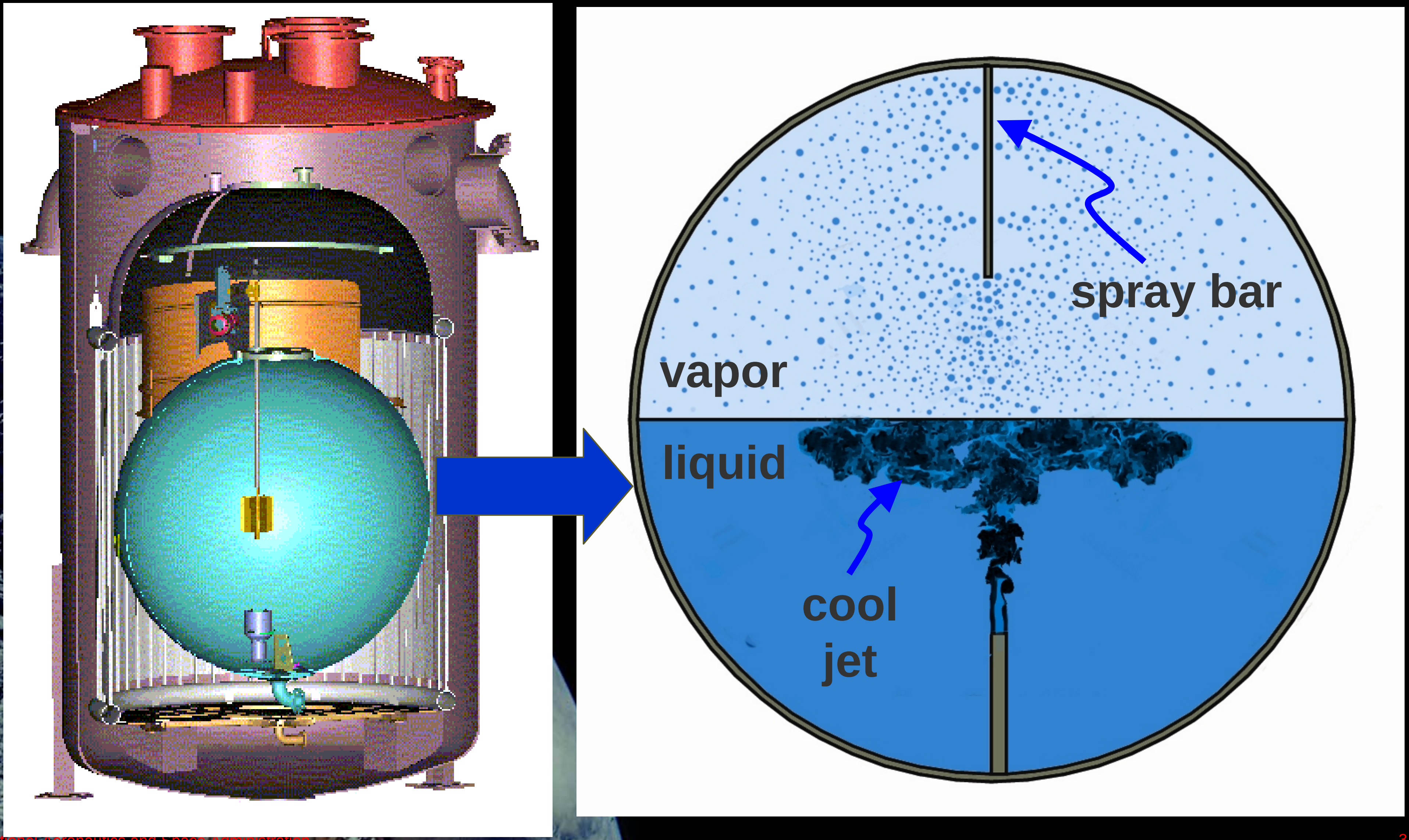
To challenge our physical understandings

To predict behavior in new situations

The purpose of this talk is to show how we can do that …

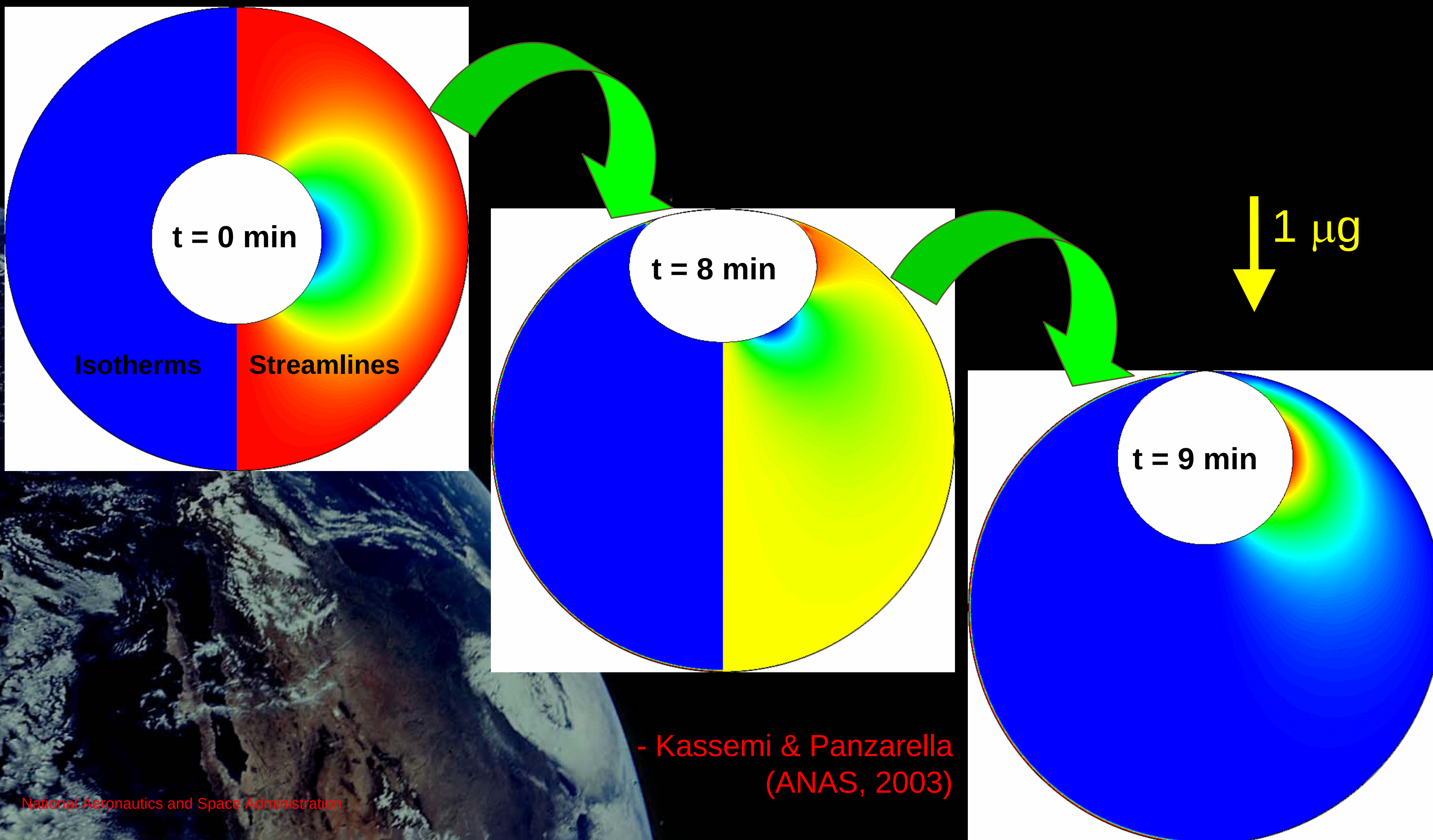
Case study: Cryogenic fuel storage

Objective: control tank pressure in space



Effect of microgravity on vapor phase

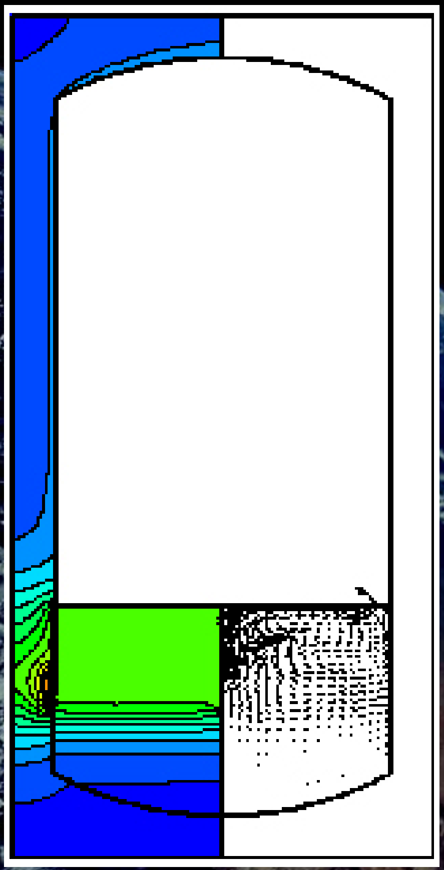
Now let's consider microgravity, in which the shape of vapor regions are dominated by surface tension, not buoyant forces

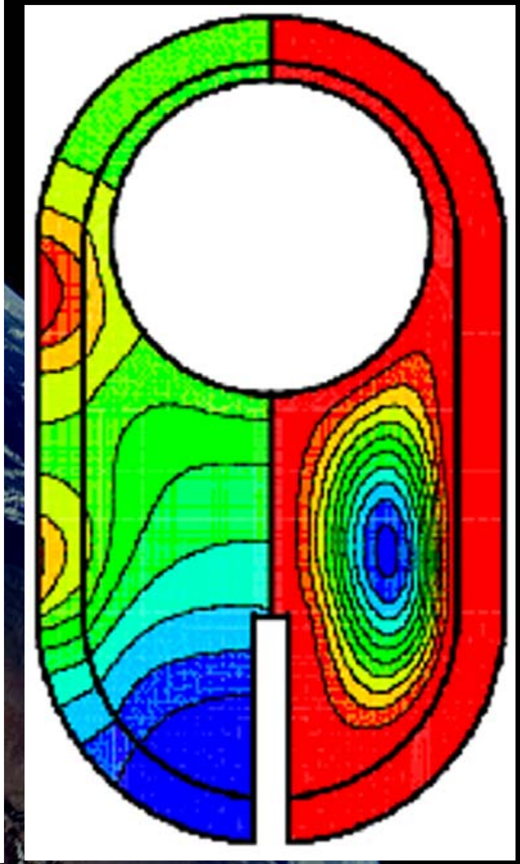


- Kassemi & Panzarella (ANAS, 2003)

What happens with a heat leak?

- With applied heat flux, there can be a pressure transient at startup that is unpredicted by bulk thermodynamics
- Using thermodynamics alone results in a persistent underprediction of tank pressure
- We would not be happy about that in space





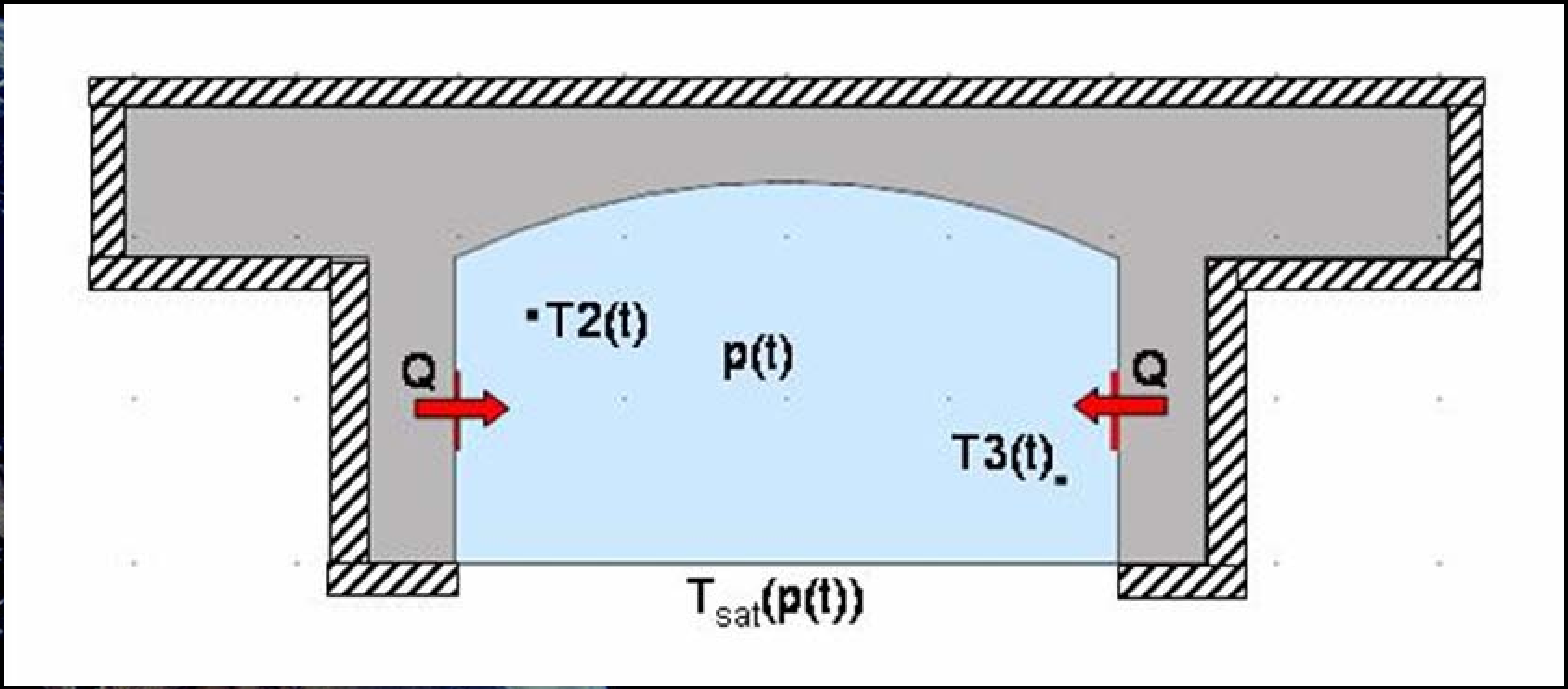
- Controlled experiments can be coupled with numerical models of increasing fidelity
  - Lumped thermodynamics
  - Lumped vapor, active liquid
  - Active vapor
  - Active vapor, active liquid, moving interface

\- Barsi & Kassemi (2006, 2008)

Active vapor model of ground-based experiments

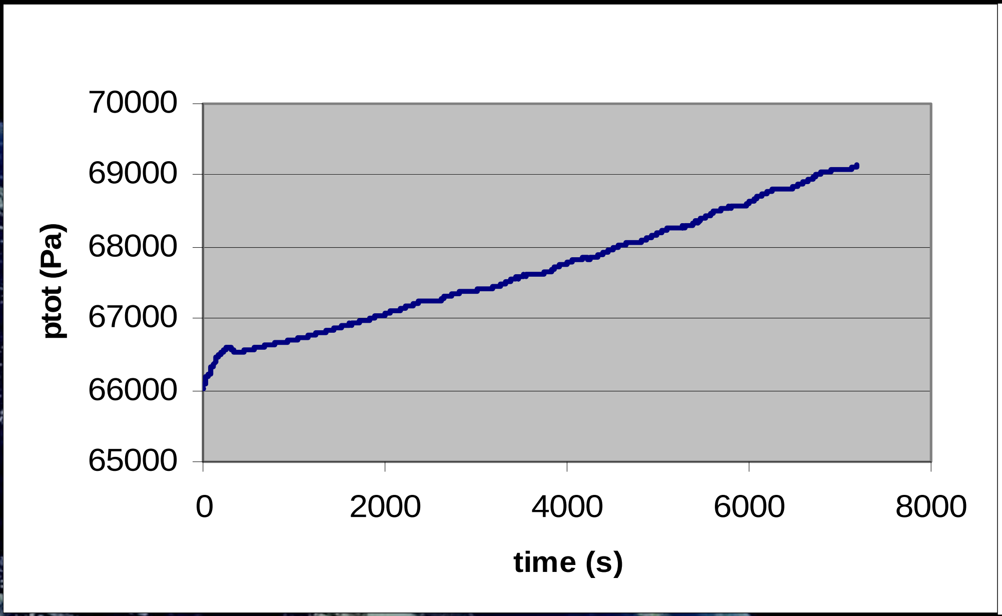
Zero Boil-Off Tank model

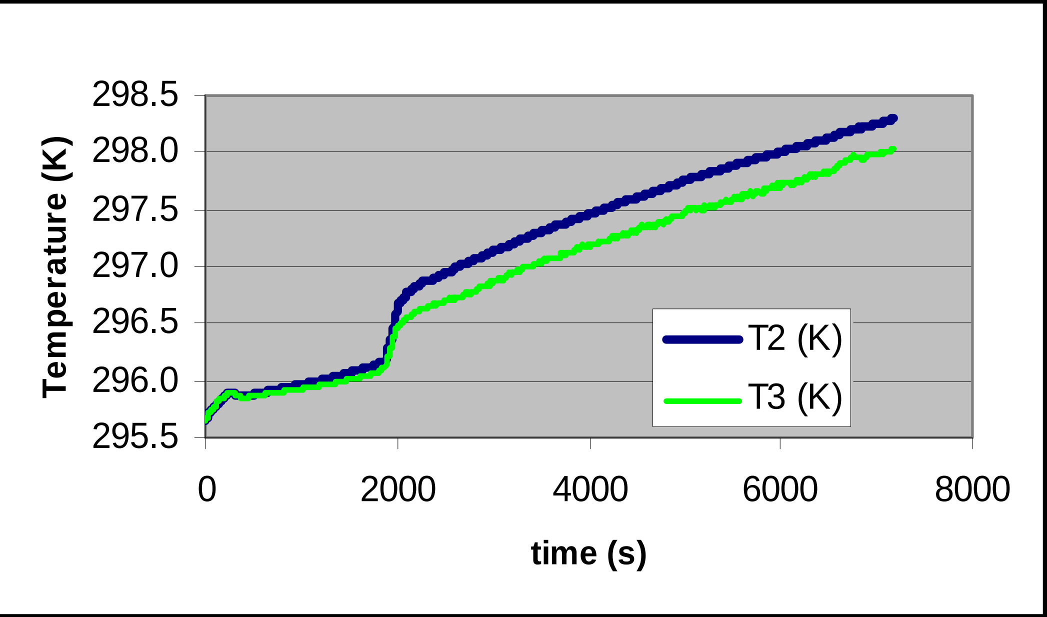
- Experiment is a transparent furnace with ring heaters and a model fluid at a variety of fill levels
- Data include p(t), and temperature histories in some cases
- Liquid/vapor interface temperature is calculated from measured pressure using the saturation curve and applied as a time-dependent boundary condition

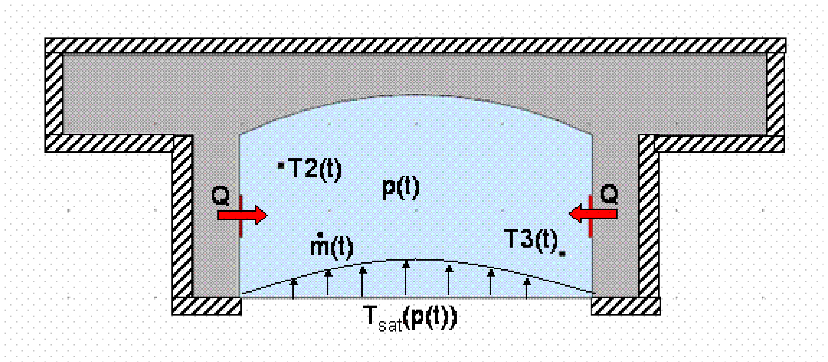


ZBOT (cont'd)

- Pressure and temperature curves from the experiment showed some shenanigans, so we set out on a series of numerical simulations to try to explain the nonlinearities
- What didn't explain it: parametric studies of thermophysical properties, simplifications in tank setup, experimental uncertainties in thermistor position, axisymmetric/planar/3D geometries, up to 30% variation in heat flux







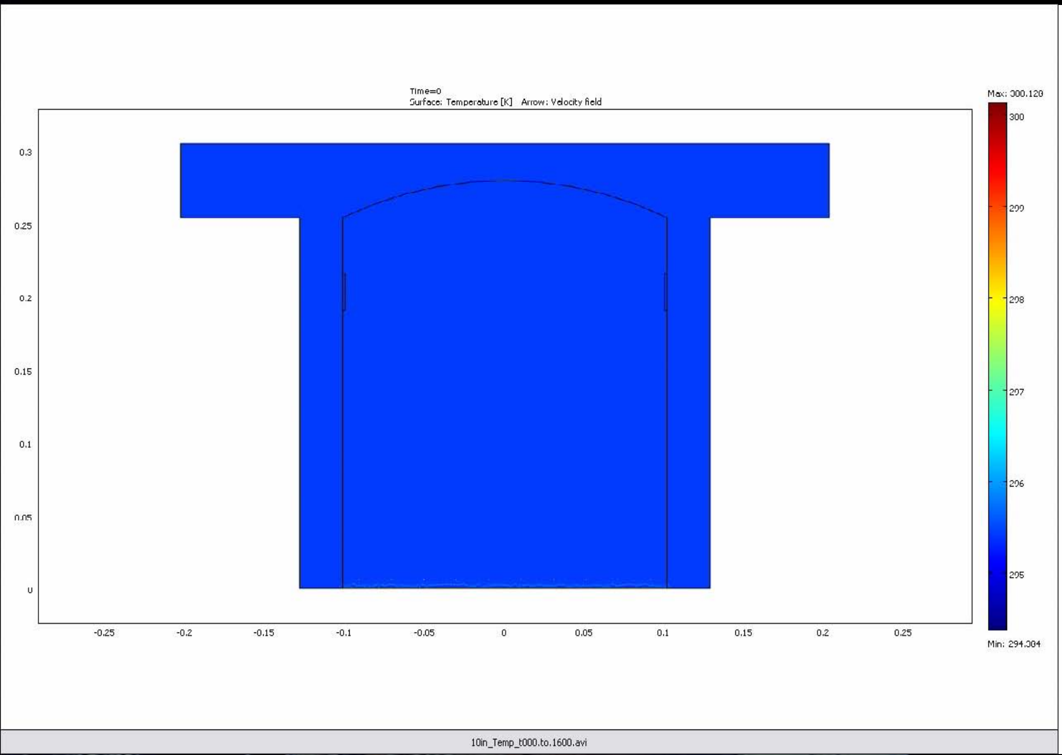
So we added new physics to incorporate compressibility and mass transfer at the interface…

Effect of mass transfer at the interface

PRELIMINARY RESULTS

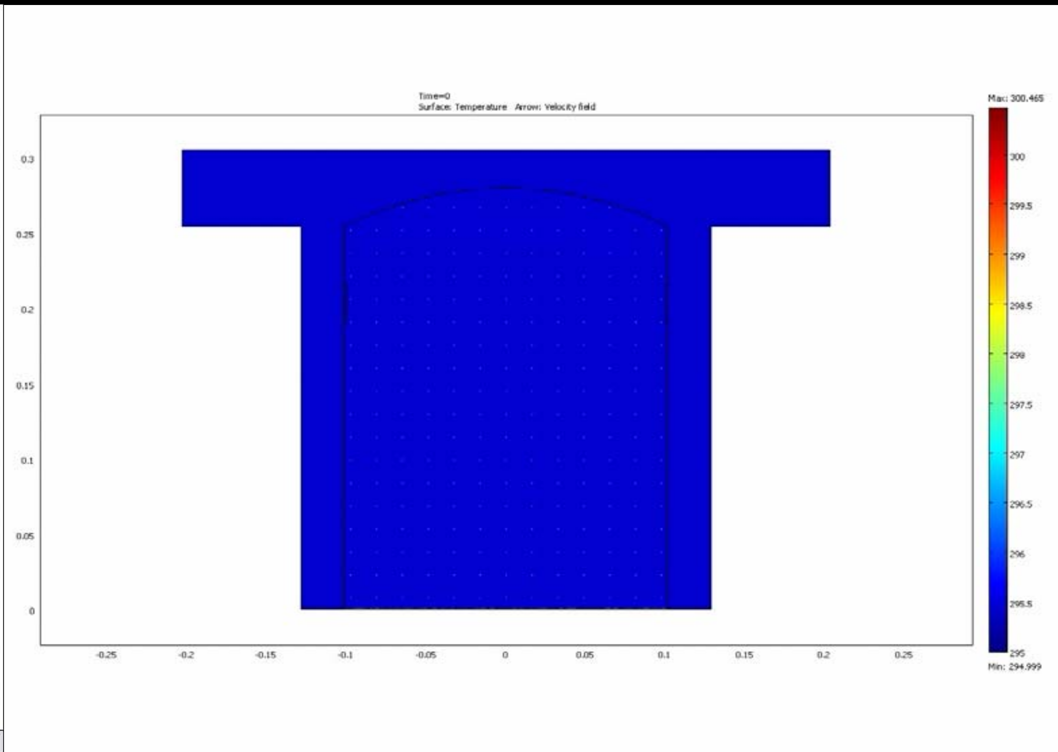
Incompressible vapor

Temperature



Compressible vapor with mass transport at interface

Temperature



… but even this isn't enough to explain it, so work continues…

Case study: Production of biofuels

Objective: Produce biofuels without impacting the food chain or the planet

- no human or animal food products
- no fresh water
- no arable land
- carbon-neutral or better

⇨ Focus on fuel from growth of salt-tolerant algae and/or cyanobacteria

Facts about algae

- Algae oil can produce aviation-grade fuel (at least in the lab)
- Algae metabolism uses CO_2 and produces O_2
- Commercial designs do not come close to their potential

Feedstock	Predicted yields (gal/acre-yr)	Current yields (gal/acre-yr)	Current production (barrels/yr)
Soybeans	50	50	>10,000,000
Sunflower	100	100	>1,000,000
Canola	160	160	>10,000,000
Palm oil	600	600	>10,000,000
Microalgae	2000-25,000	2000-?	0.1

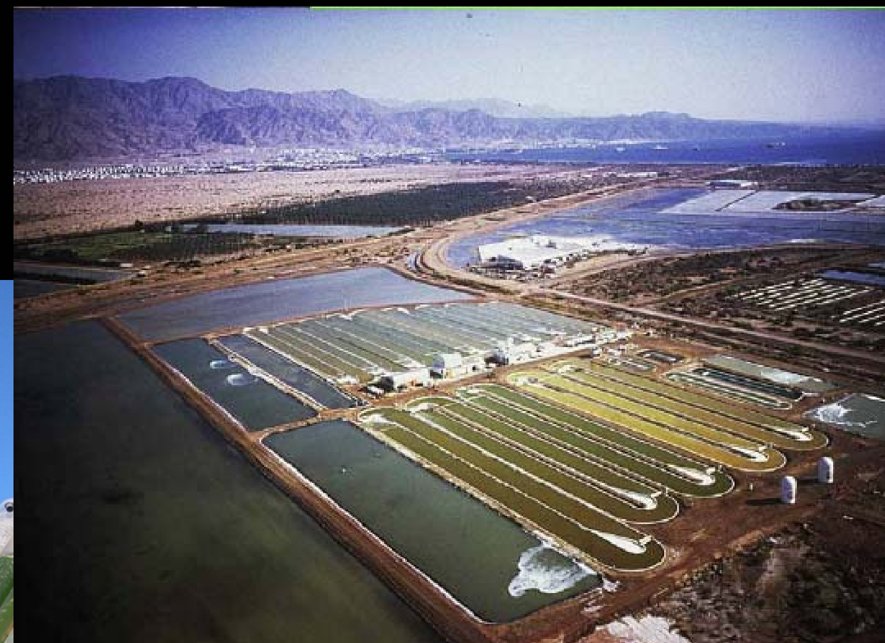
- Benemann (2007)

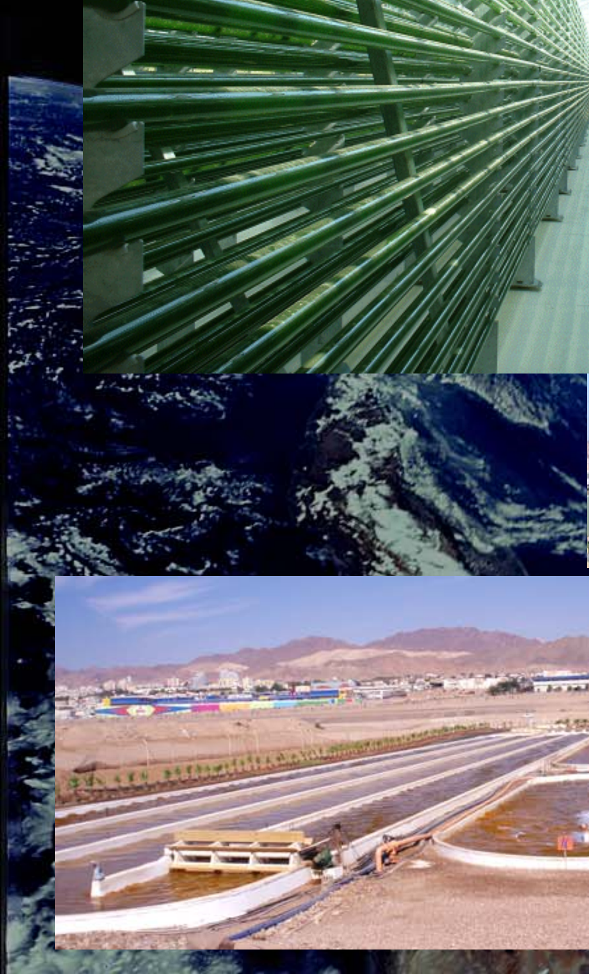
How can we improve?

- Genetic engineering is one approach to increasing yield
- Our approach is process control

Commercial algae production

- Two basic designs: closed or open





Biofuels program at GRC

Micro model(s)

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Micro-macro model

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Macro model

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Experimental Testbeds

Basic biology:

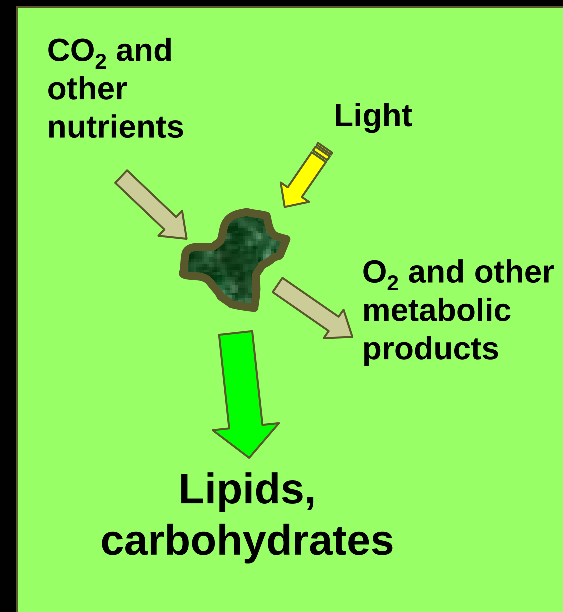
- Metabolism, energy conversion, growth, exchange w/environment

Coupling to large-scale transport:

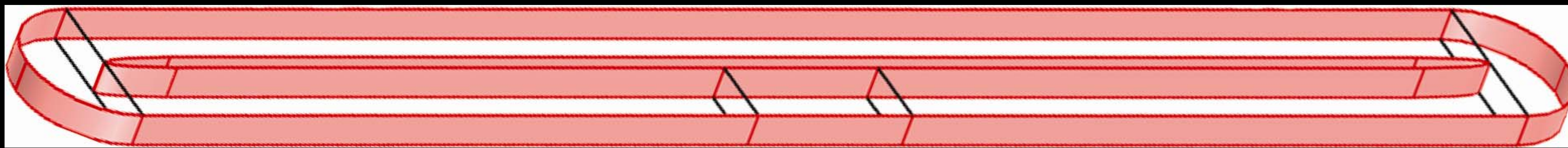
- Distribution function approach

Large scale transport processes:

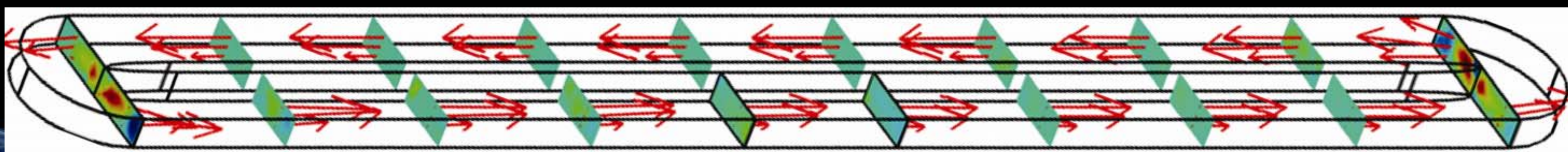
- Overall geometry, flow, nutrients
- Process optimization



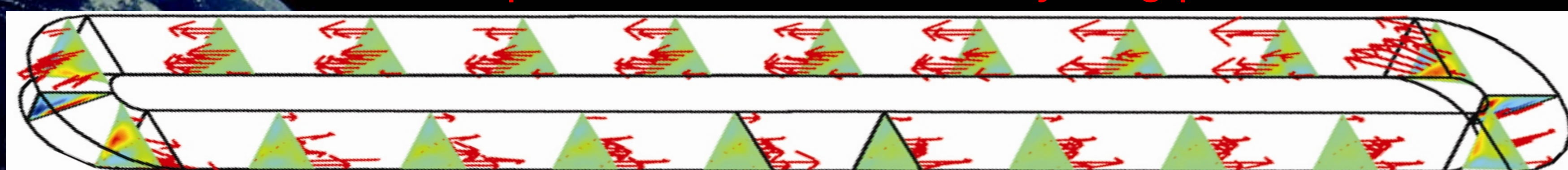
The racetrack design and simple modifications



- The basic design has not changed for decades
  - Solutions have to be *very* cheap but effective



- *Very* small vertical mixing velocities except at corners
  - This is particularly problematic due to rapid light extinction with depth and the desire for very long ponds



- Triangular cross-section buys a little, but not much
  - Passive and/or active mixers can help significantly

- LOTS of possibilities for improvement!

Conclusions

- Lessons from cryogenic tank modeling:
  - Models grow in stages from simple->complex
  - Experiments provide a reality check
  - Re the causes of p/T nonuniformities, we found what it's not
  - We may even find out what it is
  - All of the knowledge will be directly applicable to predictions of behavior in microgravity for which we have very limited data
- Lessons from biofuels:
  - Relatively simple transport models can be useful guides for process improvement
  - Lots of $$$$ impact in
    - Pond design and materials
    - Biomass yield, process time

Acknowledgements

Cryogenic fuel storage

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Biofuels

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