# REFORMER MODEL DEVELOPMENT FOR HYDROGEN PRODUCTION

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Aerospatiales

# TECHNICAL TASK, GOAL/RELEVANCE, OBJECTIVES AND TECHNICAL BARRIERS

- Technical task: "Advanced Fuel Reforming: Investigate other reformer improvements, including heat integration and reactor configuration"

- Relevance: address the goal "Research and develop low cost, highly efficient hydrogen production from…renewable sources

- Objectives: "Reduce the cost of distributed production of hydrogen from… liquid fuels"

- Technical barriers
  - A: "Reformer efficiencies are limited by side reactions"
  - A: "Improve performance"
  - H: "Hydrogen produced from biomass is not currently cost-competitive with gasoline due to … capital costs"
  - H: "Areas for reforming technology improvements include … reactor configuration for improved yield"

# METHOD OF APPROACH

- Develop models free of empiricism, as much as possible  use fundamental principles

- Sequence of the approach

    - Resolve all scales of the flow in a small domain to understand the physics (Direct Numerical Simulations (DNS)) of the drop/flow interaction, etc.

    - develop small-scale models (SGS) based on the understanding of that interaction

    - develop a model (Large Eddy Simulation (LES)) and code where we resolve only the large scales and model the small scales according to SGS

    - validate the model with experimental data

- Exercise these models to derive information directly applicable to the situation to be studied.

# PROJECT TIMELINE

Reformer model; FY02

1. Models of small-scale drop/turb-flow interactions for SC* drops; FY02
   ↓
   Evaluate small-to-large scale interact. models for SC* drops; FY03

2. Test MC*-drop model robustness for drop/turb-flow interactions; FY02 (Post Doc; PRF spons. to Bellan)
   ↓
   Develop and evaluate robust single MC*-drop model; FY03 (PRF and ONERA co-spons.)

3. New paradigm for drop injection to improve mixing; FY02 (grad. student with Egyptian fellowship)

*SC ≡ single-component

*MC ≡ multi-component mixture

# SUCCESS CRITERIA AND EXPECTED COMPLETION

- Success criteria
  - validate models with experiments
  - predict the importance of various parameters
  - optimize reforming for a laboratory scale reactor
  - predict scaling up of the reactor
- Expected completion date depends on the yearly allocated funds for the project

# ACCOMPLISHMENTS SINCE THE LAST REVIEW

- Analyzed the database created for temporal mixing layers laden with single-component drops and derived small-scale models of drops/flow interaction ("Consistent Large Eddy Simulation of a temporal mixing layer laden with evaporating drop. Part 1: Direct Numerical Simulation, formulation and *a priori* modeling", (N. Okong'o and J. Bellan), submitted to the *J. Fluid Mech*., 2002)

- Analyzed the database created for temporal mixing layers laden with multi-component drops ("Direct numerical simulation of a transitional temporal mixing layer laden with multicomponent-fuel evaporating drops using continuous thermodynamics", (P. C. Le Clercq and J. Bellan), submitted to the *J. Fluid Mech.*, 2002); found that the multi-component drop model is not robust at all far field conditions

- Developed a robust model for isolated multi-component drop evaporation ("A statistical model of multicomponent-fuel drop evaporation for many-droplet gas-liquid flow simulations", (K. G. Harstad, P. C. Le Clercq and J. Bellan), submitted to the *AIAA J*, 2003)

# ACCOMPLISHMENTS SINCE THE LAST REVIEW, cont'd

- Completing the modeling of the coupling between small-scale models and computed large-scales for single-component evaporating drops (in preparation: "Consistent Large Eddy Simulation of a temporal mixing layer laden with evaporating drops. Part II: *a posteriori* modeling", (A. Leboissetier, N. Okong'o and J. Bellan); to be submitted to the *J. Fluid Mech.*, 2003)

- Initiated the creation of a database for studying the interaction of multi-component drops with turbulent flow in a mixing layer, using the robust multi-component drop model

# SIGNIFICANT INTERACTION AND COLLABORATION WITH COLLEAGUES

- Publication: "Direct Numerical Simulations of Two-phase Laminar Jet Flows with Different Cross-Section Injection Geometries", (H. Abdel-Hameed and J. Bellan), *Phys. Fluids*, 14(10), 3655-3674, 2002; published in the NASA Tech Briefs => available to the broader community

- Three additional papers submitted for journal publication; each to be published in the NASA Tech Briefs

- Presentations (all to be published in the NASA Tech Briefs):

  - 2 papers presented at ILASS 2002, May 2002

  - 1 paper presented at the 41st Aerospace Sciences Meeting, January 2003

  - 2 papers presented at the 3rd Joint US Sections Combustion Institute Meeting, March 2003

# SIGNIFICANT INTERACTION AND COLLABORATION WITH COLLEAGUES cont'd

- Proposals written with colleagues to develop additional experimental databases for model validation

  - collaboration with University of Southern California professor to develop experimental database for single-component drop sprays; submitted to NASA Microgravity Fluids, December 2002

  - collaboration with University of California Davis professor to develop experimental database for multi-component drop sprays; submitted to NASA Microgravity Combustion, March 2003

- Requests for re-prints (e.g. Prof. J. Corella from Spain, Prof. M. Papalexandris from Belgium who will visit at JPL 7/08/03)

## FUTURE MILESTONES: SPRAY WITH SINGLE-COMPONENT DROPS

Spatial spray in FY04 (instead of temporal mixing layer in FY02 and FY03)

↓

1. Laminar, evaporating spray DNS runs; FY04

↓

2. Laminar, evaporating spray LES runs; FY04

↓

3. Turbulent, evaporating spray LES and experimental validation; FY04
Data of McDonell and Samuelsen, *Atomization and Sprays*, 3, 321-364, 1993; others

# FUTURE MILESTONES: TEMPORAL MIXING LAYER WITH MULTI-COMPONENT DROPS

Temporal mixing layer with robust multi-component-drop model; FY04

↓

1. Creation of the DNS database; FY04

↓

2. Initiation of the database analysis to model the drop/small-scale interaction; FY04

## ISSUE 1 FROM 2002 REVIEWERS: MODEL USEFULNESS

- Assist in resolving important challenges in reforming:
  - reduction of coke formation: the current emphasis on $\nearrow$ steam/carbon ratio is a global strategy whereas coke is formed locally
  - temperature optimization: $\nearrow T$ leads to more conversion, but it also leads to $\nearrow CO/CO_2$ ratio due to the reverse water-gas shift reaction
  - single-chemical-species diesel-surrogates or pyrolysis-oil surrogates behave differently than diesel or pyrolysis oil $\Rightarrow$ ensure that experiments are performed with diesel or pyrolysis oil instead of surrogates
  - investigate the optimal $T$ range resulting from diesel-fuel or pyrolysis-oil composition variation
  - predict the chemical species distribution $\Rightarrow$ location of the catalyst
  - predict how reformers will scale up from the micro-reactors used in laboratories

# ISSUE 2 FROM 2002 REVIEWERS: EFFORT TO MAKE THE WORK ACCESSIBLE TO THE BROAD COMMUNITY

- LES is an engineering approach supported by scientific (i.e. DNS) results: The analysis of the DNS database to

    - extract models for the interaction between evaporating drops and turbulent flow

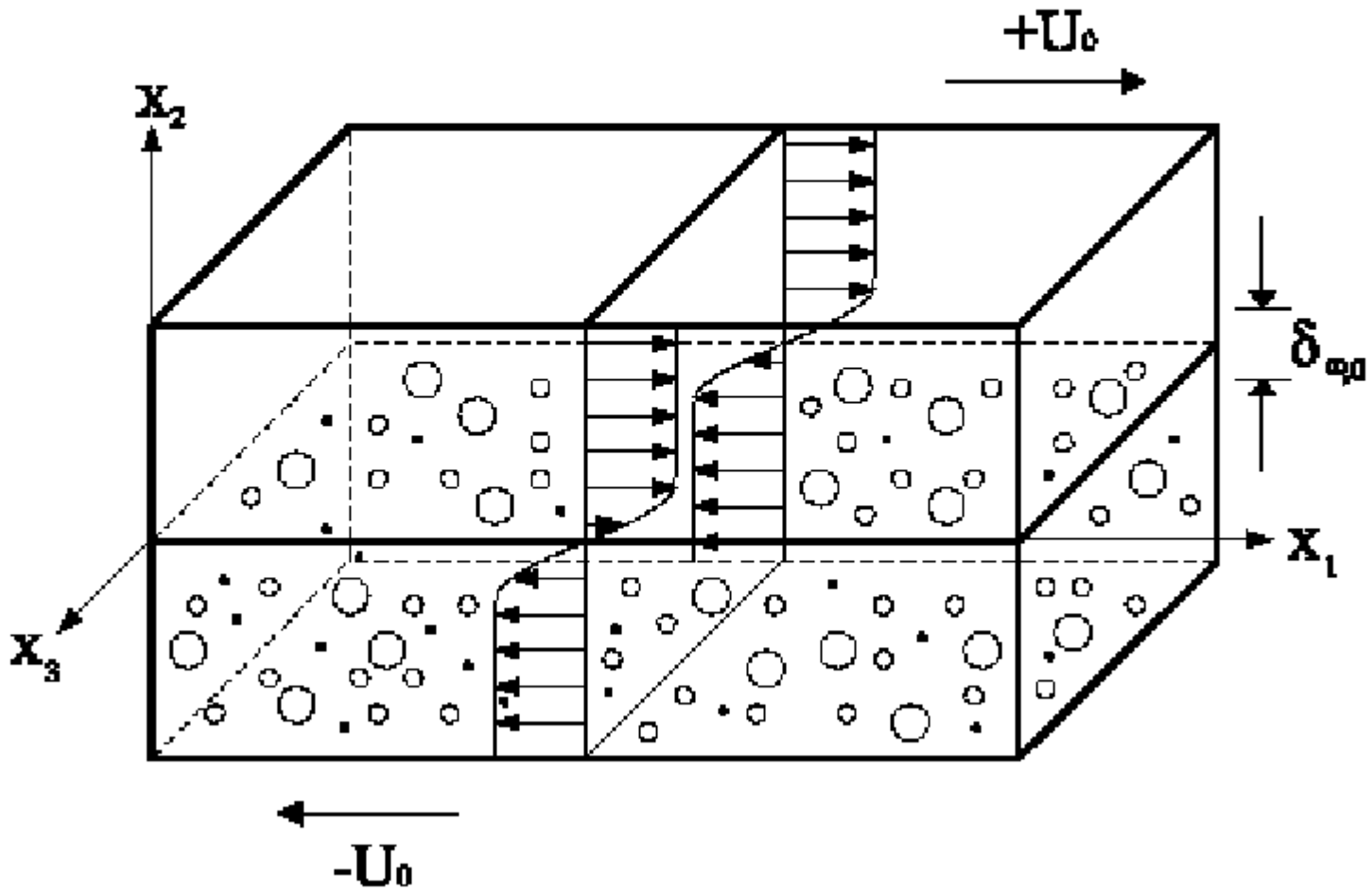
    - reduce the tracked number of drops while maintaining accuracy

make the problem computationally tractable and thus accessible to the broader community. JPL obtained a reduction by a factor of $10^2$ in computational time while retaining good accuracy.

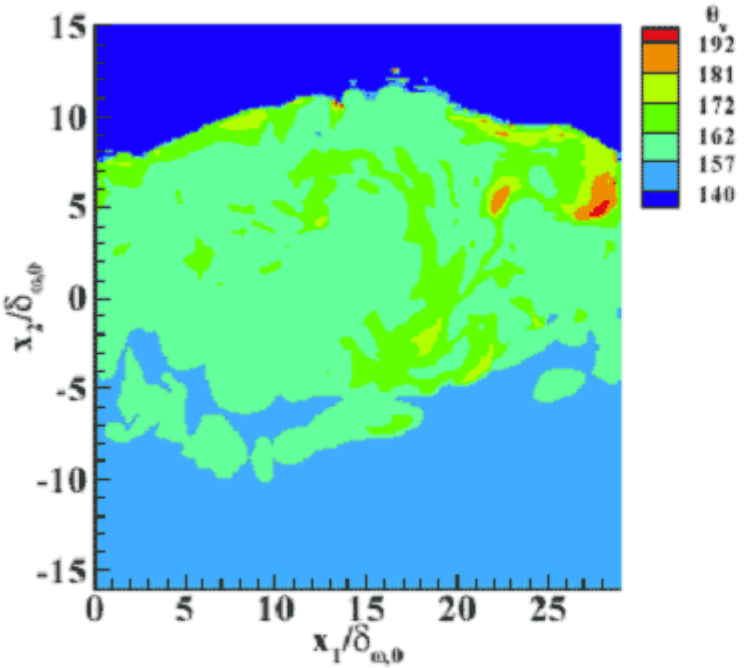
- Idea of the DNS/SGS/LES is to compute only the larger scales, and model the small scales => computational efficiency

- NASA Tech Briefs (all papers under the $H_2$ Program sponsorship) make the work available to the broader community

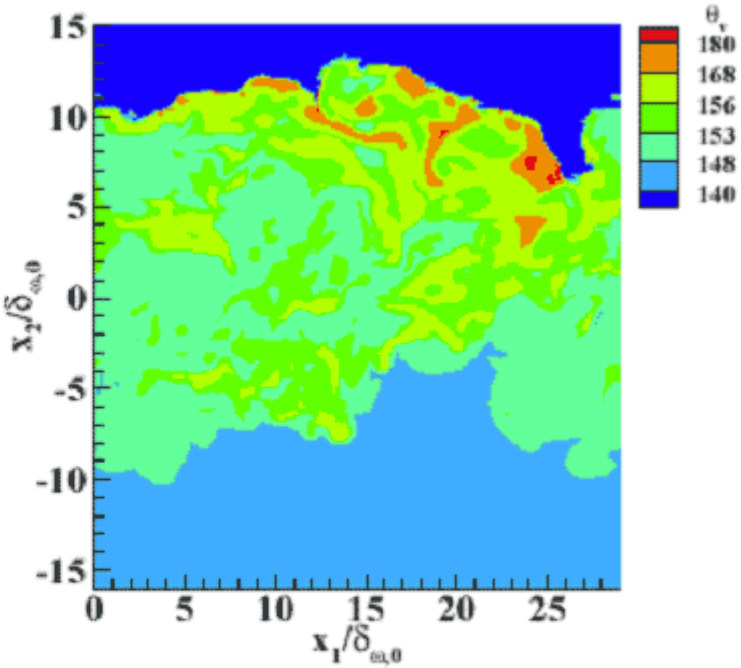
# MIXING LAYER CONFIGURATION



# BETWEEN-THE-BRAID PLANE CONTOURS OF THE MEAN MOLAR WIGHT FOR EVAPORATING DIESEL FUEL




$ML_0 = 0.2$



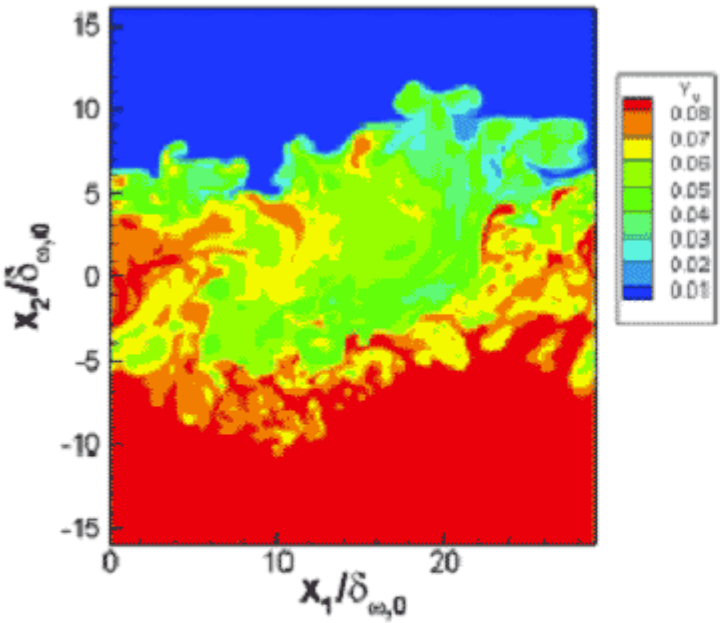

$ML_0 = 0.5$

$ML_0$ is the initial mass loading of the layer.

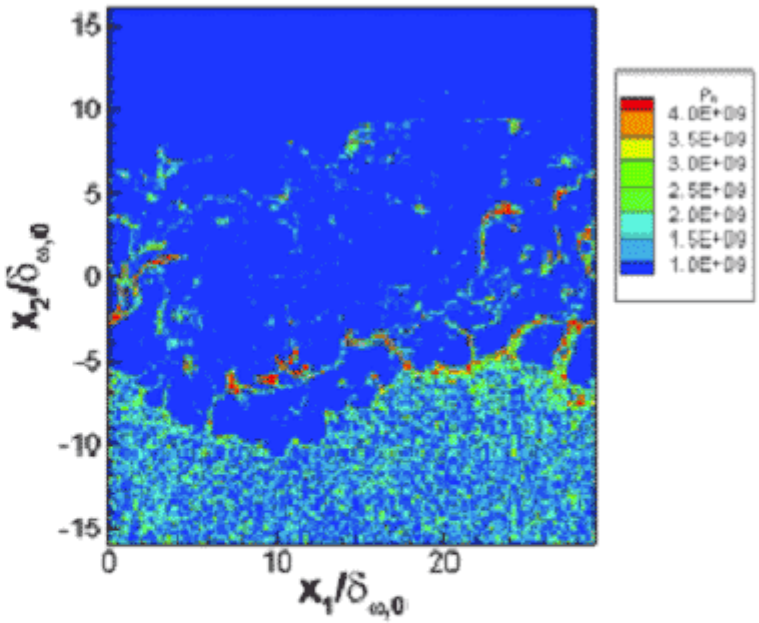
For single-component drops the mean molar weigh is uniform in the field. This shows the importance of doing experiments and performing simulations with the real fuel rather than a single-chemical-species surrogate.

# BETWEEN-THE-BRAID PLANE CONTOURS OF THE VAPOR MASS FRACTION AND DROP NUMBER DENSITY

## DNS WITH ALL DROPS; 2252 CPU HOURS




vapor mass fraction

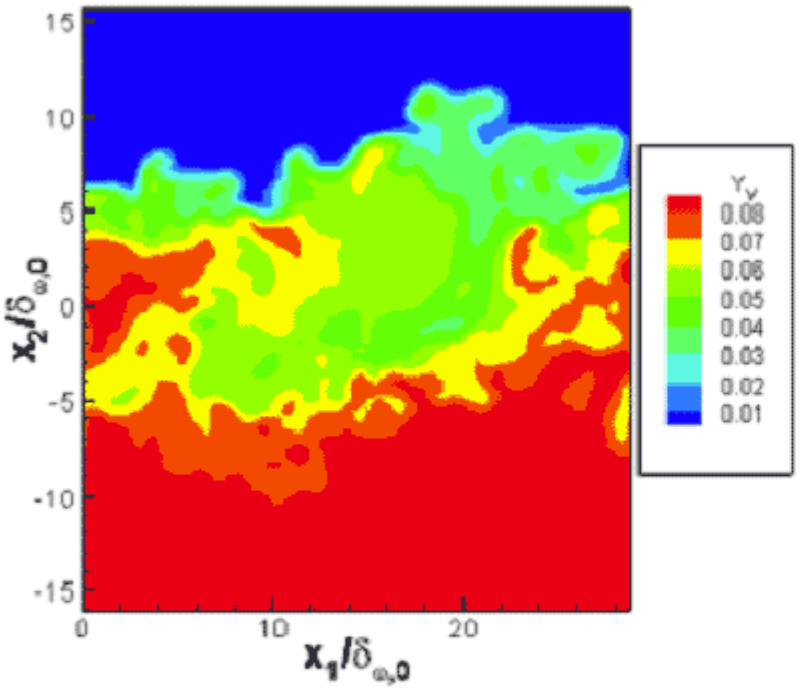



drop number density ($m^{-3}$)

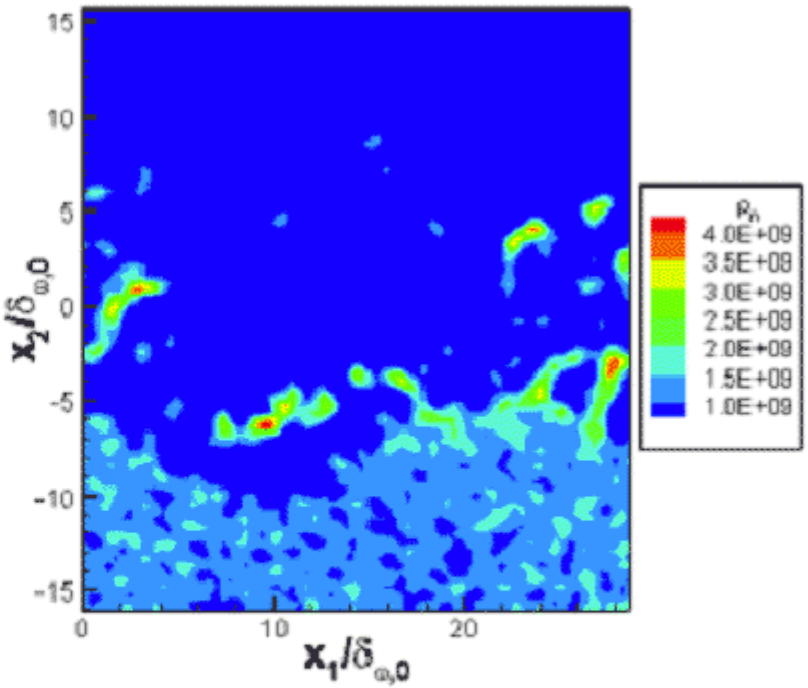
Simulation for $ML_0 = 0.2$.

# BETWEEN-THE-BRAID PLANE CONTOURS OF THE VAPOR MASS FRACTION AND DROP NUMBER DENSITY

## FILTERED AND COARSENED DNS AND OLY 1 OUT OF 8 DROPS PORTRAYED




vapor mass fraction

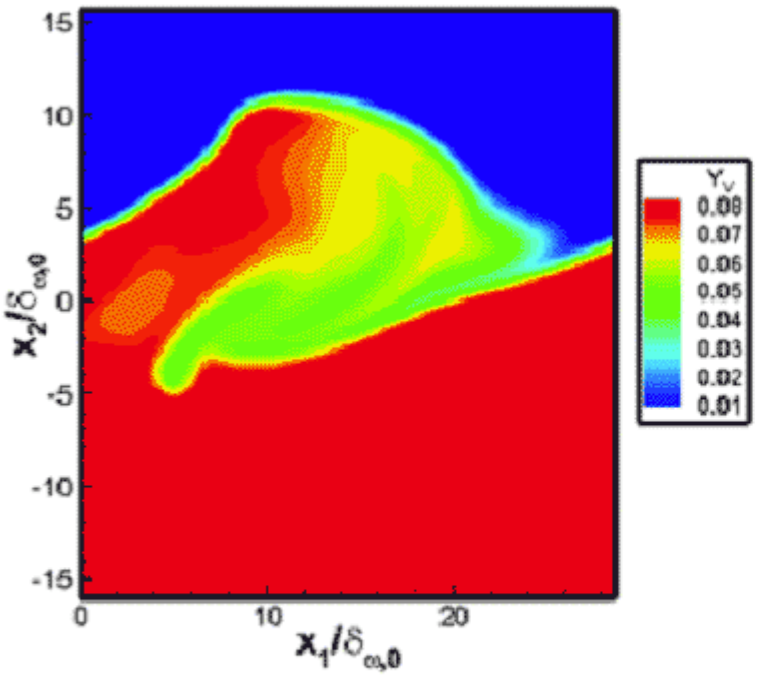



drop number density ($m^{-3}$)

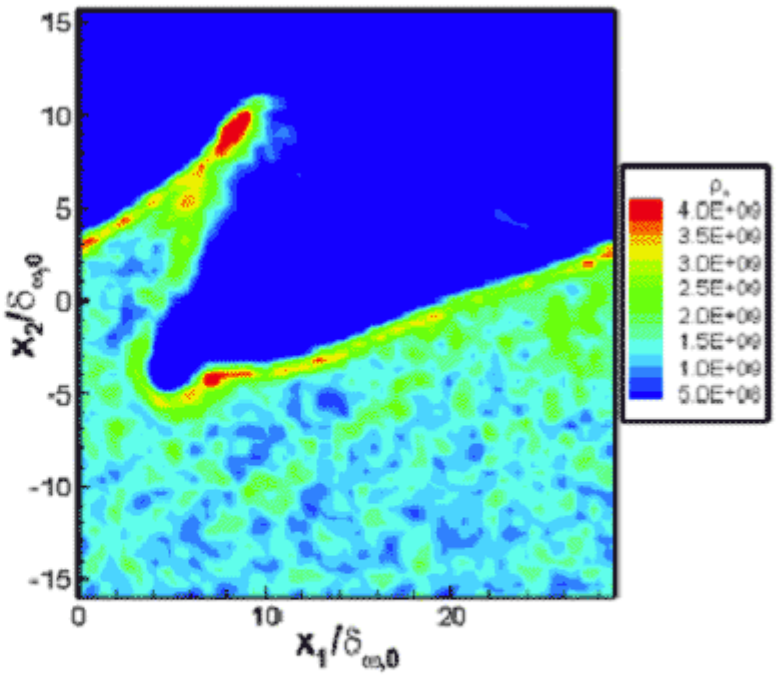
Simulation for $ML_0 = 0.2$.

# BETWEEN-THE-BRAID PLANE CONTOURS OF THE VAPOR MASS FRACTION AND DROP NUMBER DENSITY, cont'd

## TYPICAL SMALL-SCALE (ie MIXING LENGTH) MODEL USED IN ENGINEERING CALCUATIONS AND ONLY 1 OUT OF 8 DROPS CONSIDERED IN THE SIMULATION; 20.1 CPU HOURS




vapor mass fraction

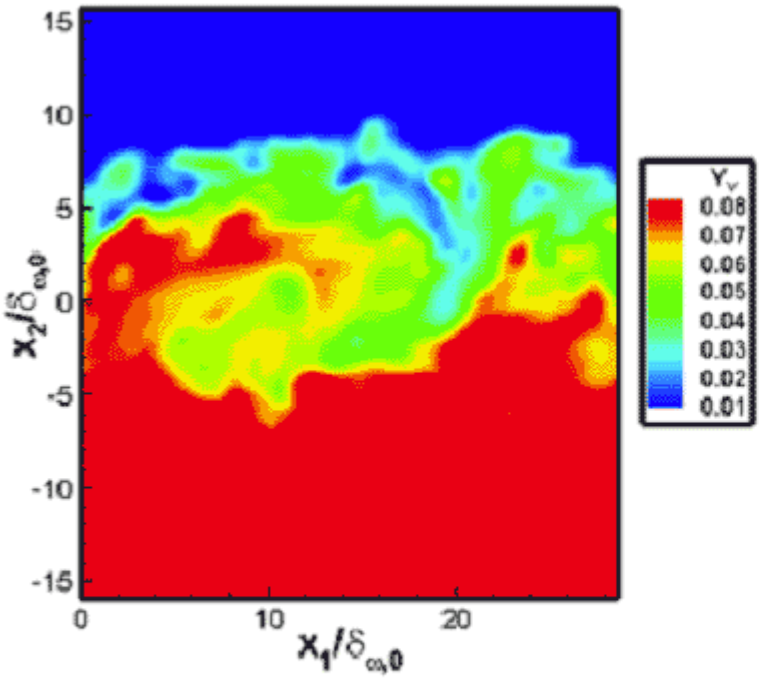



drop number density ($m^{-3}$)

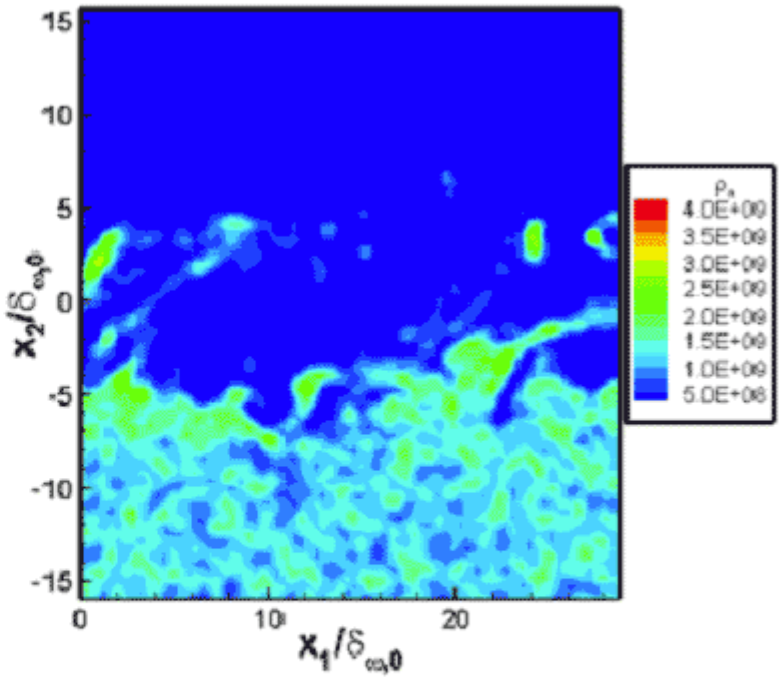
Simulation for $ML_0 = 0.2$.

# BETWEEN-THE-BRAID PLANE CONTOURS OF THE VAPOR MASS FRACTION AND DROP NUMBER DENSITY, cont'd

## JPL-DEVELOPED MODEL AND ONLY 1 OUT OF 8 DROPS CONSIDERED IN THE SIMULATION; 19.8 CPU HOURS




vapor mass fraction

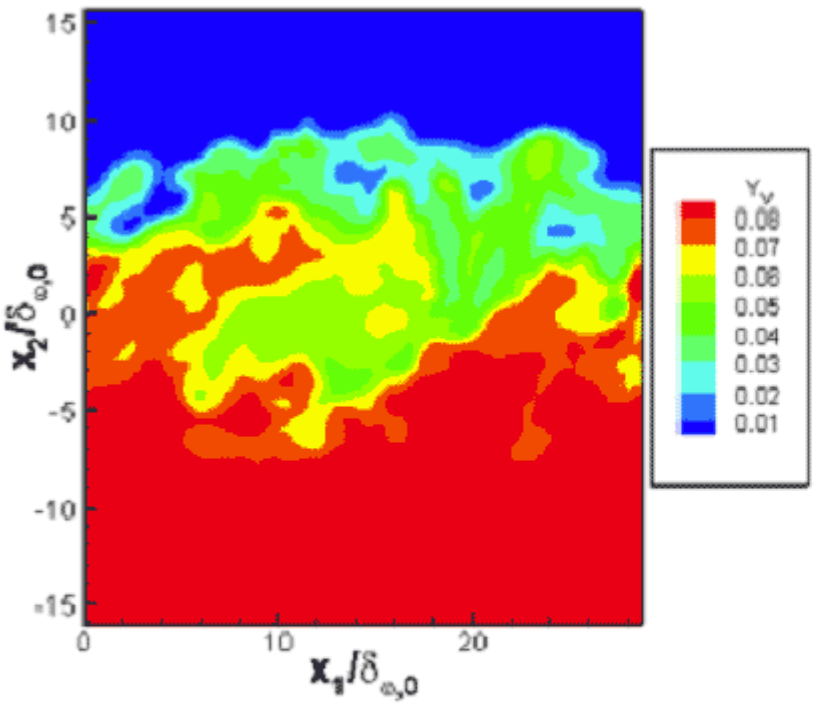



drop number density ($m^{-3}$)

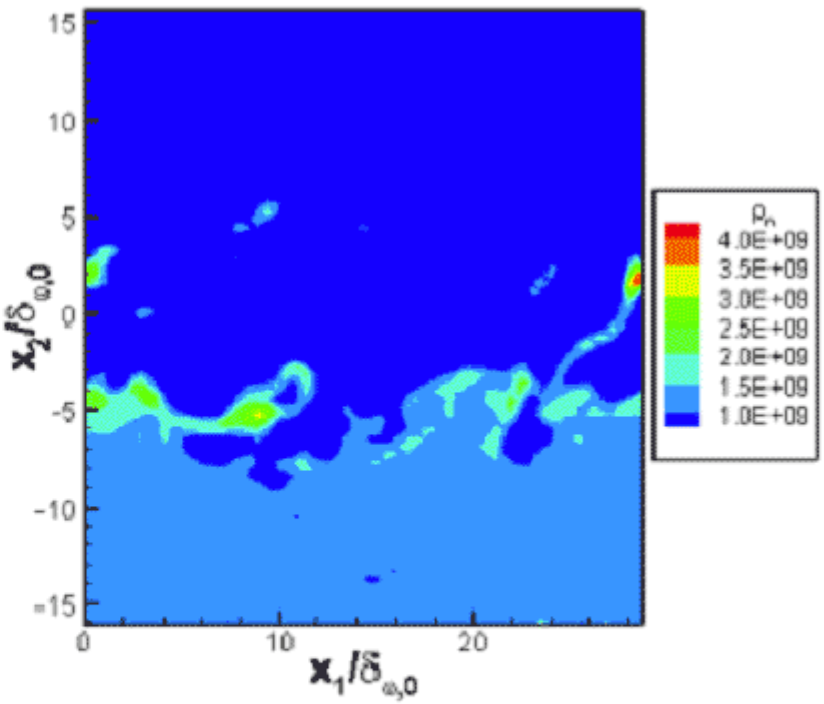
Simulation for $ML_0 = 0.2$.

# EFFECT OF THE NUMBER OF DROPS

## JPL-DEVELOPED MODEL WITH ALL DROPS; 113 CPU HOURS




vapor mass fraction



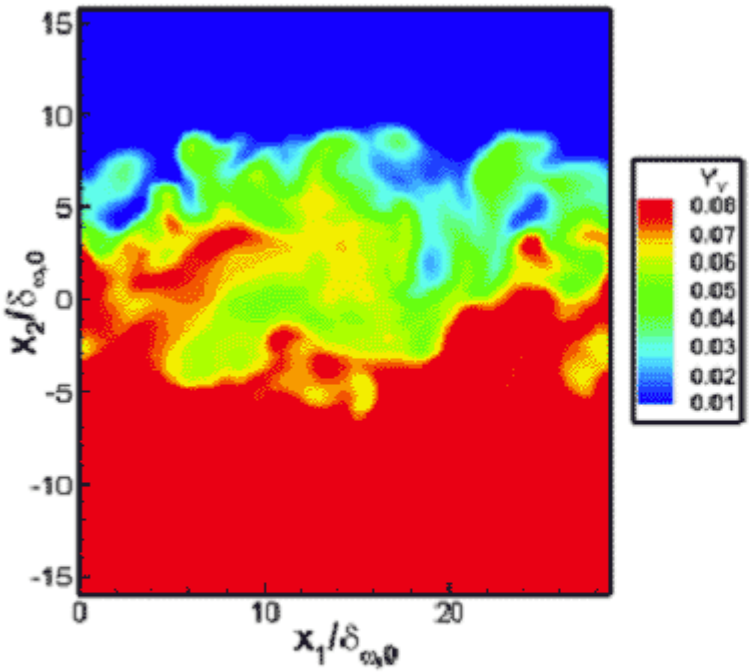

drop number density ($m^{-3}$)

Simulation for $ML_0 = 0.2$.

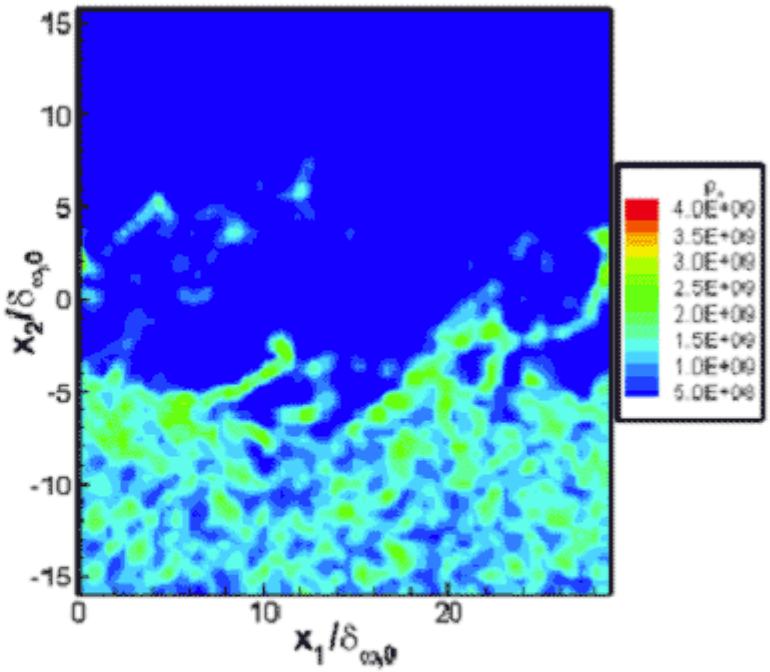
# EFFECT OF THE NUMBER OF DROPS, cont'd

## JPL DEVELOPED MODEL WITH ONLY 1 OUT OF 16 DROPS

## 12.2 CPU HOURS




vapor mass fraction



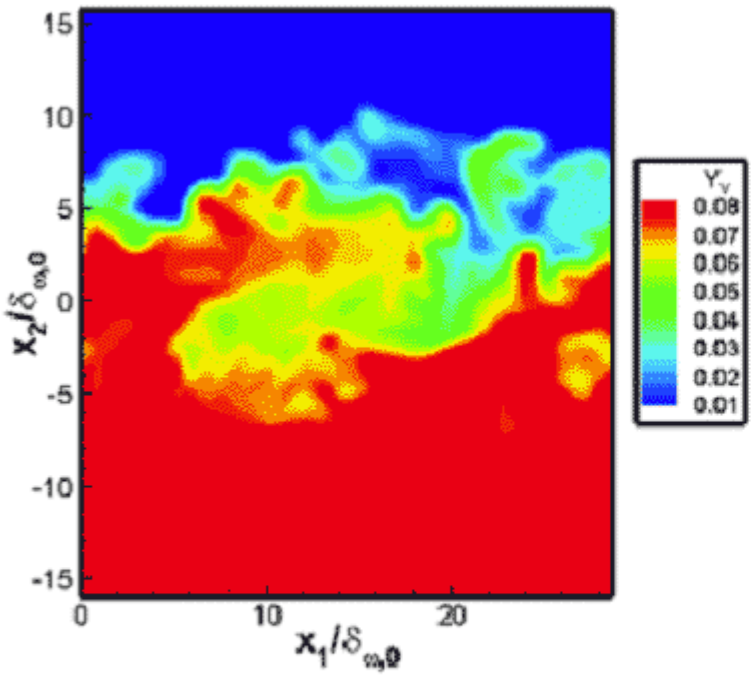

drop number density ($m^{-3}$)

Simulation for $ML_0 = 0.2$.

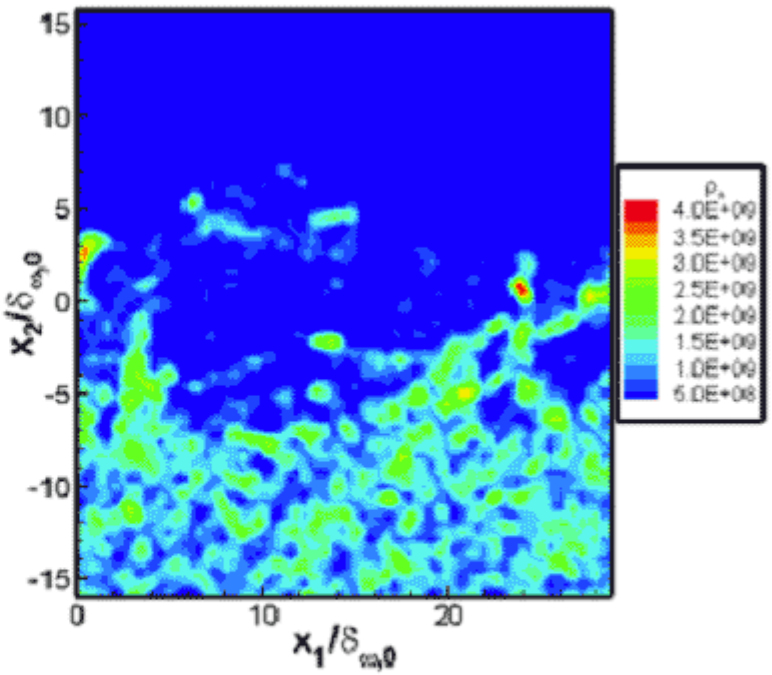
# EFFECT OF THE NUMBER OF DROPS, cont'd

## JPL DEVELOPED MODEL WITH ONLY 1 OUT OF 32 DROPS

## 9.4 CPU HOURS




vapor mass fraction



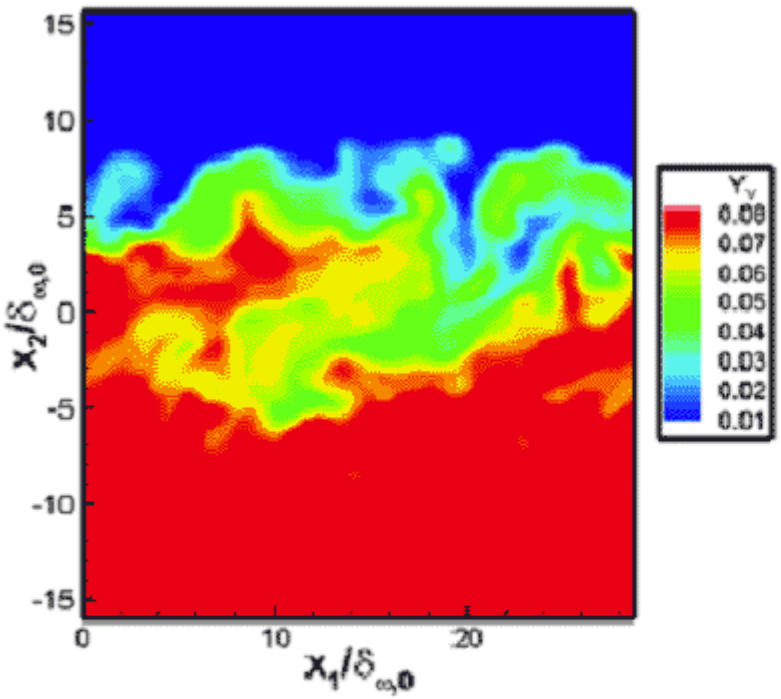

drop number density ($m^{-3}$)

Simulation for $ML_0 = 0.2$.

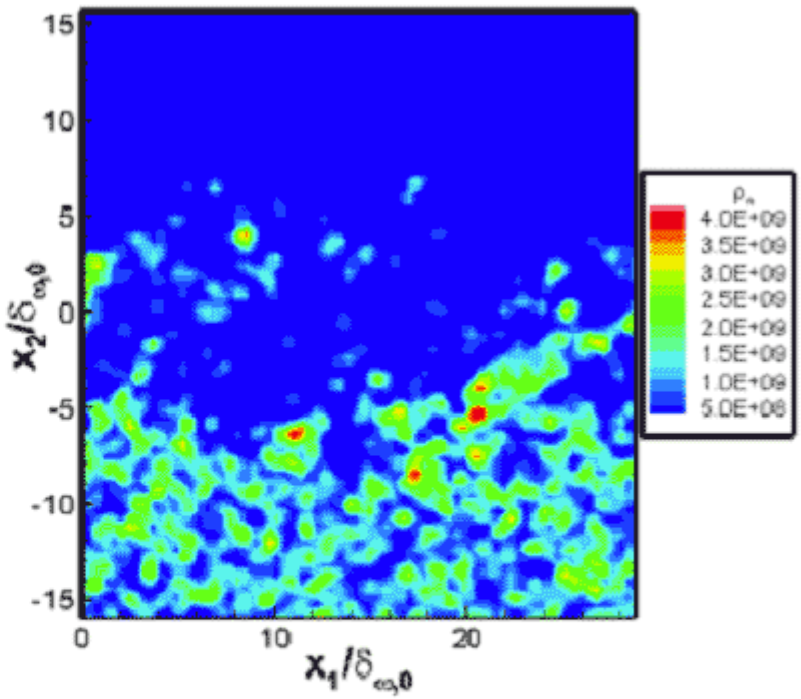
# EFFECT OF THE NUMBER OF DROPS, cont'd

## JPL DEVELOPED MODEL WITH ONLY 1 OUT OF 64 DROPS

## 8.1 CPU HOURS




vapor mass fraction




drop number density ($m^{-3}$)

Simulation for $ML_0 = 0.2$.