Modeling of polydisperse sprays using a high order size moment method for the numerical simulation of advection and evaporation

Damien KAH, Marc MASSOT (ECP),
Frédérique LAURENT (CNRS), Stéphane JAY (IFP)

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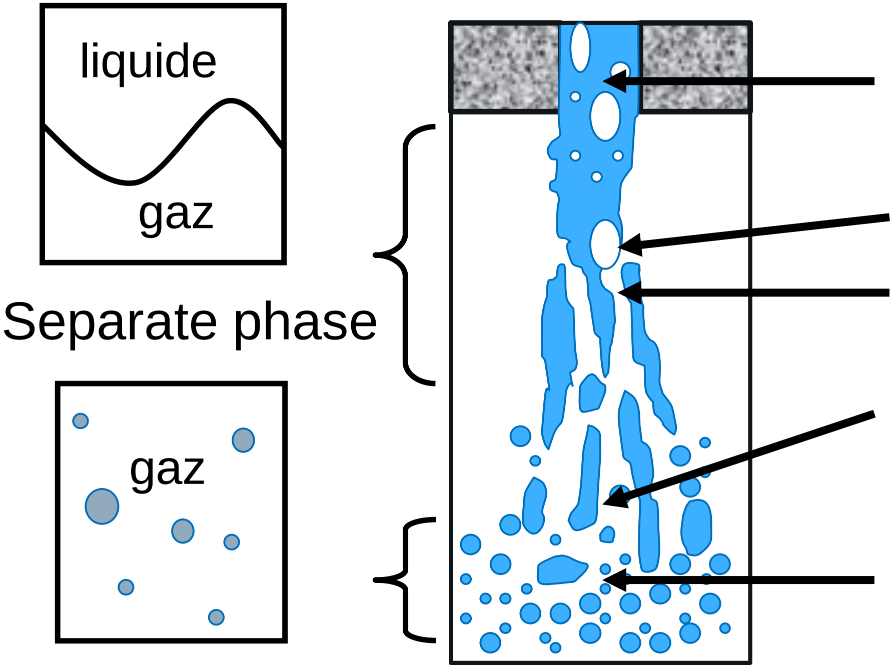
General context: injection in engines

- Sprays in internal combustion engines
- Numerical simulation of reactive multiphase flow



- Cavitation
- Primary atomization
- Turbulence in surrounding gas due to drag force exerted by the liquid
- Secondary atomization
- Evaporation, drag, heat exchange
- Collisions, coalescence

Dispersed and dilute phase

General context: modeling of two-phase flow

- Two ways of modeling

- **Lagrangian**
  - Implementation
  - Coupling gas/liquid
  - Non stationary flow: high CPU cost

- **Eulerian**
  - Coupling gas/liquide
  - Non stationary flow
  - Modeling, Implementation

- Current modeling (IFP-C3D): **Euler/Euler** version (*Truchot 05, Vessiller 08, Bayoro 08*)
  Baer et Nunziato model *(85)*
  - *7* equation model
  - Mixture, interface, cavitation, detonation

Our objective

- Improve the description of the coupling terms (gas/liquid)

⇨ Better predict fuel fraction in gas for combustion solvers (Temperature, NOx,…)

  - Separate phase: evolution of interfacial area Σ *(Jay 06)*
  - Dispersed phase: description of **polydispersity**

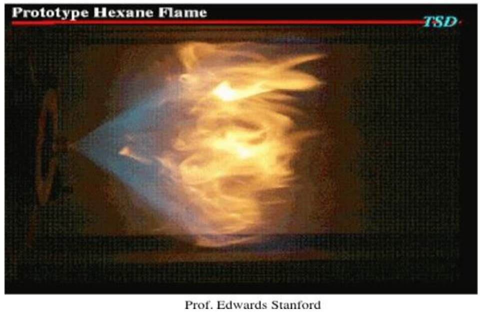


Fig: Prof Edwards (Stanford)

- IFP-C3D : two-fluid formalism
  - Volume fraction : α
  - Interfacial area density : Σ

Mean diameter : $d = \frac{6\alpha}{\Sigma}$

- How to introduce the capacity to describe polydispersity in the dispersed phase, in a two-fluid formalism ?

Description of polydispersity(1/2)

- Statistical approach
  - Spherical droplets (1-100 µm): no interface problem
  - Number density function (NDF) $f(t, x, v, S, T)$
  - Williams-Boltzmann Equation (*Williams, 1958*)

$$\boxed{\partial_t f + \partial_x v f + \partial_S R f + \partial_v \frac{F}{m} f + \partial_T E f = \Gamma}$$

- Eulerian framework
  - Resolution with Finite Volume impossible $\Rightarrow$ moment method
  - Size moments $m_k = \int_0^{S_{max}} \int_{\mathbb{R}} S^k f \, dS dv$

- Models describing polydispersity in a Eulerian framework ?

Description of polydispersity(2/2)

- Sectional method (*Tambour 1985*) : Multi-fluid method (*Laurent 02, Chaisemartin 09*)
  - Several size sections $[S_i, S_{i+1}]$
  - Evolution of $m_{3/2,i}, m_{3/2,i}u_i$ in each section
  - Can describe every distribution function
  - High accuracy potential
  - Important CPU cost, at least 2 sections to describe polydispersity
- Two-fluid formalism: Presumed NDF method (*Mossa 05*)
  - One section
  - Presumed NDF, not generical
  - Scheme not stable for evaporation

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What we precisely want to achieve

- Design a method
  - Describing polydispersity in a two-fluid formalism
  - Generic
  - Reasonnable CPU cost

$\Rightarrow$ **Several size moments**

- Difficulties :
  - **Mathematic**: closure problems
  - **Physics** : accuracy of the description ?
  - **Numerical** : stable scheme

- Different contexts, solved independtly through splitting :
  - Evaporation
  - Advection in physical space

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- Advection
- Conclusions - Perspectives

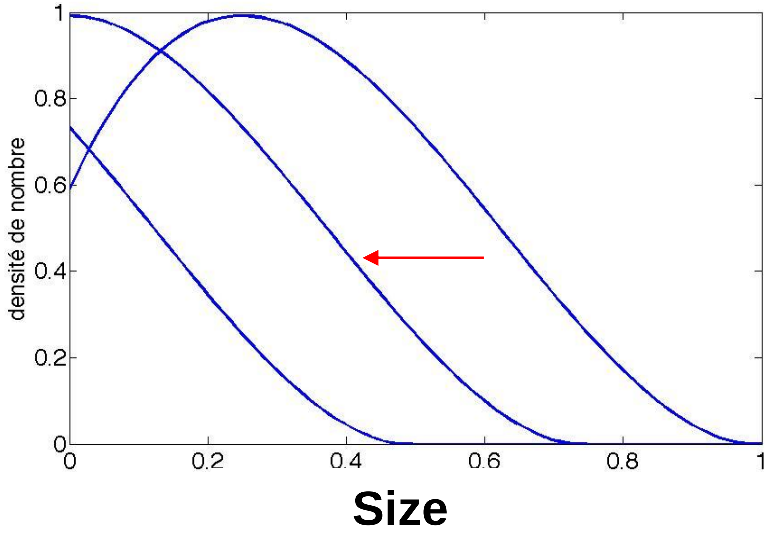
Evaporation: Principle

- Solution of $\partial_t f + \partial_S R f = 0$
- R, evaporation coefficient, determined by an evaporation model
- We use d² law (infinite conductivity)

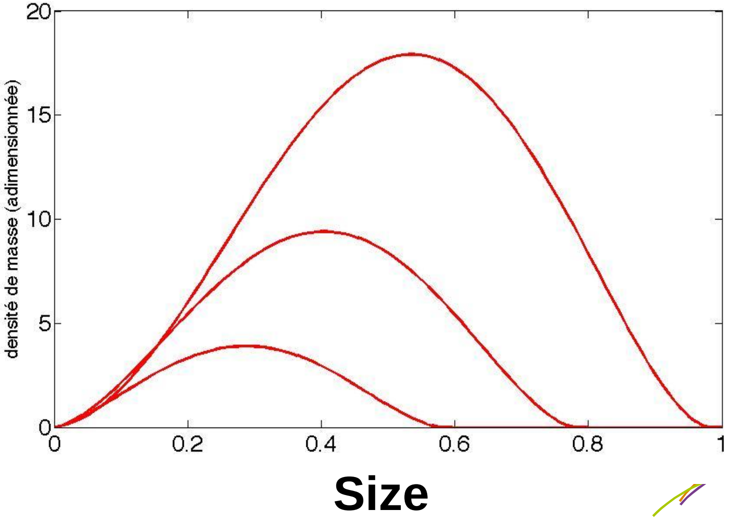
  and non dimensional variables: $R = -1, S \in [0, 1]$

Analytical solution

Density



Mass Density



Evaporation: Model

- $\partial_t f + \partial_S (Rf) = 0$ phase space: S
- $\int_0^1 \int_{\mathbb{R}} S^k \partial_t f \, dS dv + \int_0^1 \int_{\mathbb{R}} S^k \partial_S (Rf) \, dS dv = 0, \; k = 0 \ldots 3$
- Dynamics of four size moments:

m_0: number density

m_1: mean size

m_2: mean square size, dispersion around the mean value

m_3: mean cubic size

Evaporation: Model

- $\partial_t f + \partial_S (Rf) = 0$
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- $\partial_t m_0 =$ **- *f(t,S=0)*: evaporative flux**

$$\partial_t m_1 = -m_0$$

$$\partial_t m_2 = -2m_1$$

$$\partial_t m_3 = -3m_2$$

Evaporation: Model

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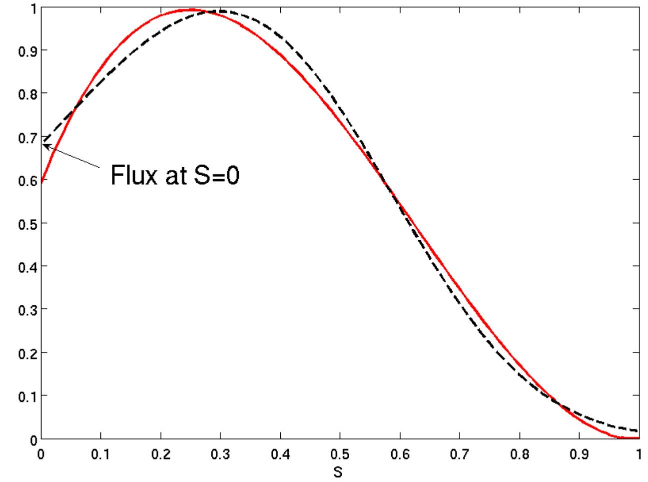


Feasibility (Moments of a NDF)
(Fox,Laurent,Massot 08)

⇒ **Entropy Maximisation** *(Mead 84)*

Evaporation: Numerical scheme

- ODE solvers are unstable: Explicit Euler, 2 stage Runge Kutta.
- New scheme
  - Finite Volume scheme
  - Flux calculation by temporal integration of the kinetic equation

  Equivalence microscopic / macroscopic description levels (*Bouchut 03*)

  $\partial_t f$ $\qquad\qquad$ $\partial_t m_k$

- Algorithm
  - Moments in the section
  - Reconstruction of *f* by Entropy Maximisation
  - Calculation of the flux using *f*, solution of the kinetic equation
  - Flux addition and update of the moments

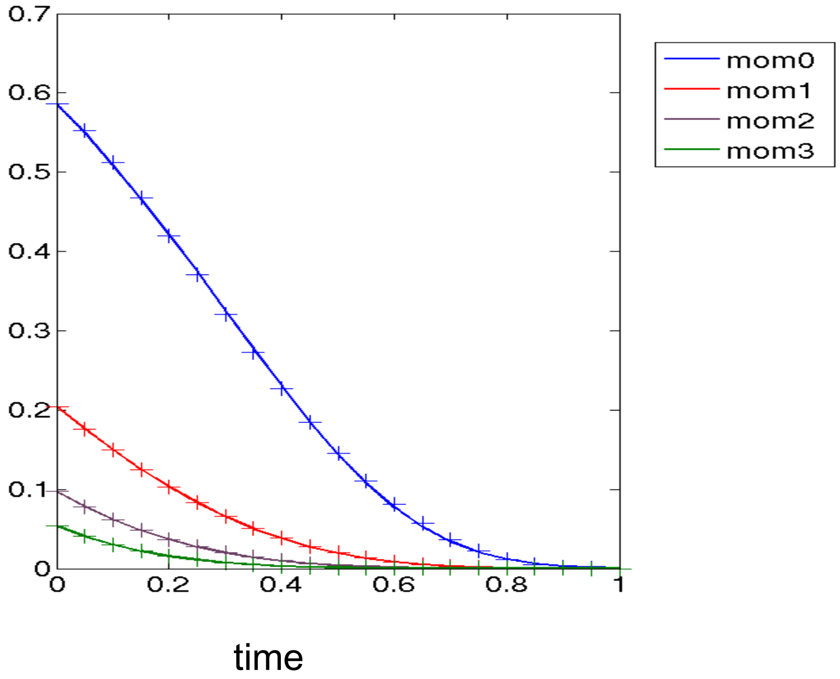
⇨ Kinetic scheme (*Perthame 02*)

Satisfies the feasability condition

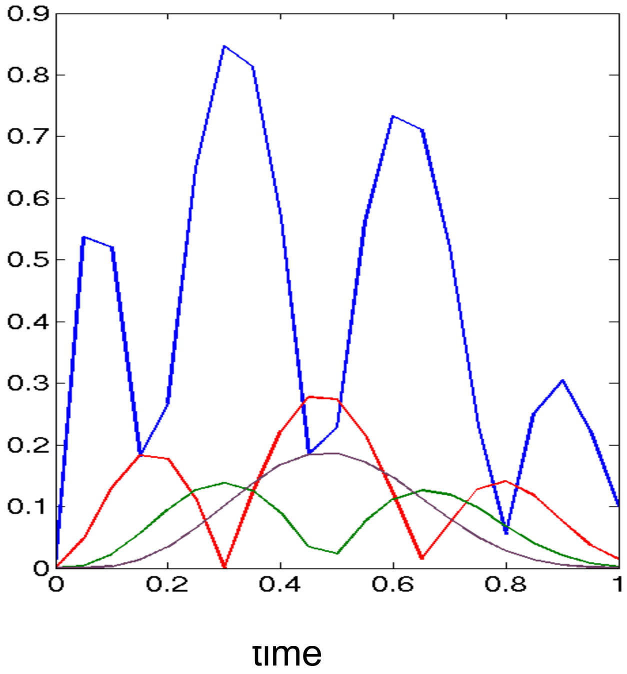
Evaporation: Results

Results in terms of moments

- Analytical and numerical moments



- Error on the moments (in percent)



Good accuracy of the method

Evaporation: Conclusion

- $$\partial_t f + \partial_S (Rf) = 0 \quad , \quad R = -1, S \in [0,1]$$

- Solution in terms of moments *(Massot et al 08)*
  - Closure problem: Entropy Maximisation
  - Numerical scheme: Kinetic scheme

- **Applications:**

  - Implement these evolution equations in IFP-C3D
  - New closure of the evaporation term

Ability to evaporate a population with different sizes

- Application in other domain: soots

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Advection: model (1/2)

- $\partial_t f + \partial_x (v f) = 0$ phase space : (S,v)
- $\int_{\mathbb{R}} \partial_t (\begin{pmatrix} 1 \\ v \end{pmatrix} f) \, dv + \int_{\mathbb{R}} \partial_x (\begin{pmatrix} v \\ v^2 \end{pmatrix} f) \, dv = 0$ Velocity moments

Advection: model (1/2)

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closure problem

⇨ Unique velocity conditioned by size

$$f(t,x,v,s) = n(t,x,S)\delta(v - u(t,x,S))$$

Advection: model (1/2)

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closure problem

⇒ Unique velocity conditioned by size

$$f(t,x,v,s) = n(t,x,S)\delta(v - u(t,x,S))$$

- $\partial_t \int_0^1 nu \, dS + \partial_x \int_0^1 n(u)^2 \, dS = 0$ Size moments

Advection: model (1/2)

- $$\partial_t f + \partial_x(v f) = 0$$ phase space : (S,v)
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$$f(t,x,v,s) = n(t,x,S)\delta(v - u(t,x,S))$$

- $$\partial_t \int_0^1 nu\, dS + \partial_x \int_0^1 n(u)^2\, dS = 0$$ Size moments

⇨ Constant velocity in a section

$$\int_0^1 u^2(S) f\, dS = m_0 \bar{u^2} = m_0 (\bar{u})^2$$

Advection: model (2/2)

$$\partial_t m_0 + \partial_x m_0 \bar{u} = 0$$
$$\partial_t m_1 + \partial_x m_1 \bar{u} = 0$$
$$\partial_t m_2 + \partial_x m_2 \bar{u} = 0$$
$$\partial_t m_3 + \partial_x m_3 \bar{u} = 0$$
$$\partial_t m_0 \bar{u} + \partial_x m_0 \bar{u}^2 = 0$$

- Objective: Design a 2nd order scheme satisfying:

Advection: model (2/2)

$$\partial_t m_0 + \partial_x m_0 \bar{u} = 0$$

$$\partial_t m_1 + \partial_x m_1 \bar{u} = 0$$

$$\partial_t m_2 + \partial_x m_2 \bar{u} = 0$$

$$\partial_t m_3 + \partial_x m_3 \bar{u} = 0$$

$$\partial_t m_0 \bar{u} + \partial_x m_0 \bar{u}^2 = 0$$

- Objective: Design a 2nd order scheme satisfying:
- Feasability condition
  - Independant transport of the moment fails
- Presurreless Gas formalism (*Bouchut 03*)
  - Potentiel singularity formation (δ-shocks)

Pressureless Gas formalism

- $$\begin{aligned} \partial_t m_0 + \partial_x m_0 \bar{u} &= 0 \\ \partial_t m_0 \bar{u} + \partial_x m_0 \bar{u}^2 &= 0 \end{aligned}$$ **Pressure=0**

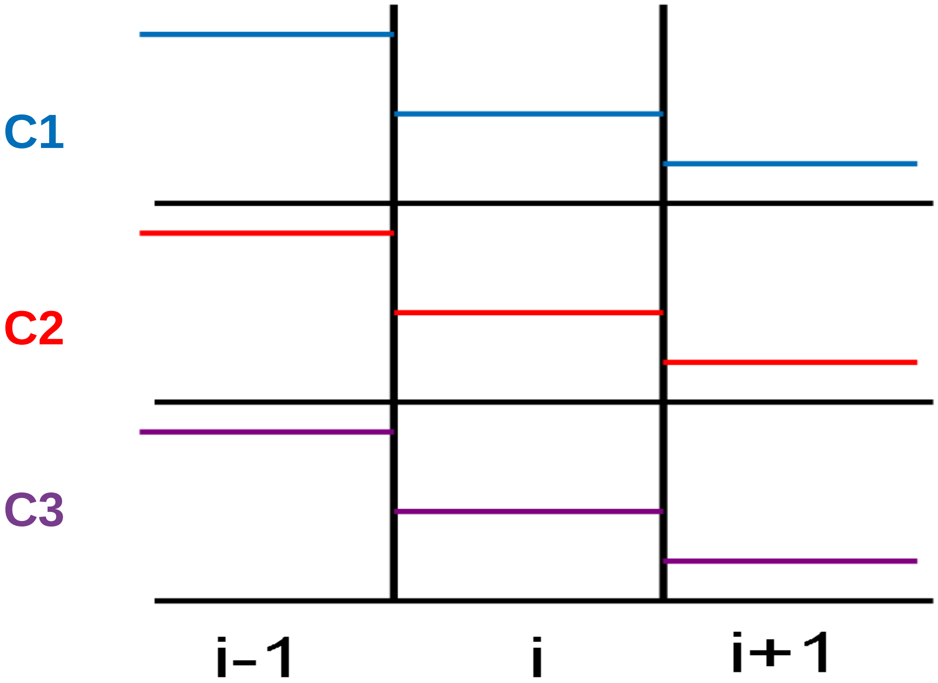
- $$\partial_t \bar{u} + \bar{u} \partial_x \bar{u} = 0$$ (Burgers Equation)

- Potential singularity formation

  Kinetic scheme

Feasability condition (1/3)

- $c_k = \dfrac{m_k}{m_0},\ k = 1..3 \Longrightarrow \partial_t c_k + u \partial_x c_k = 0$
- Reconstruction



Feasability condition (2/3)

- $c_k = \frac{m_k}{m_0},\ k = 1..3 \Longrightarrow \partial_t c_k + u \partial_x c_k = 0$
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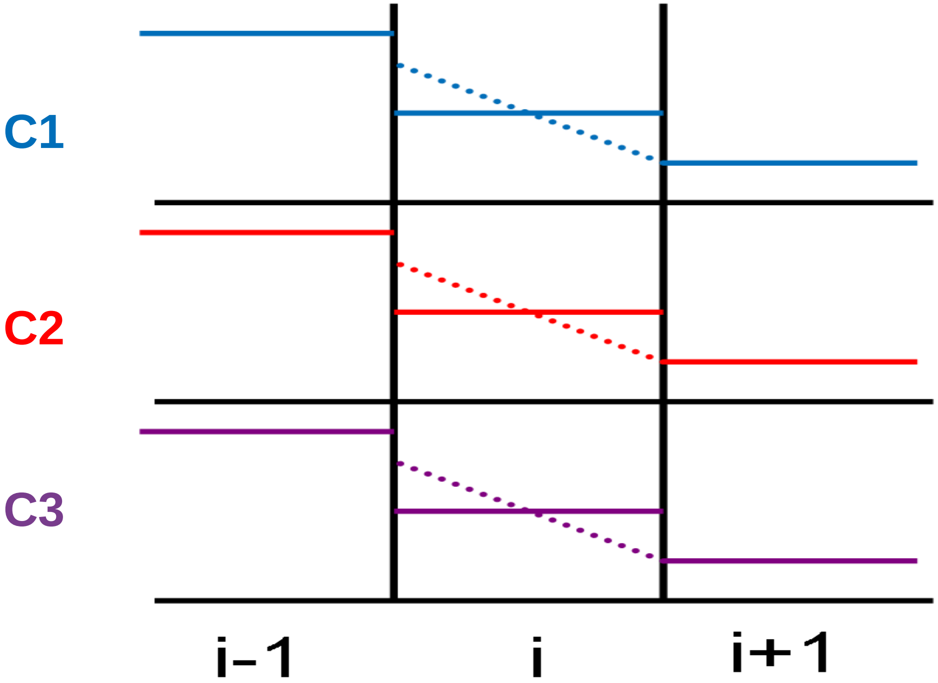
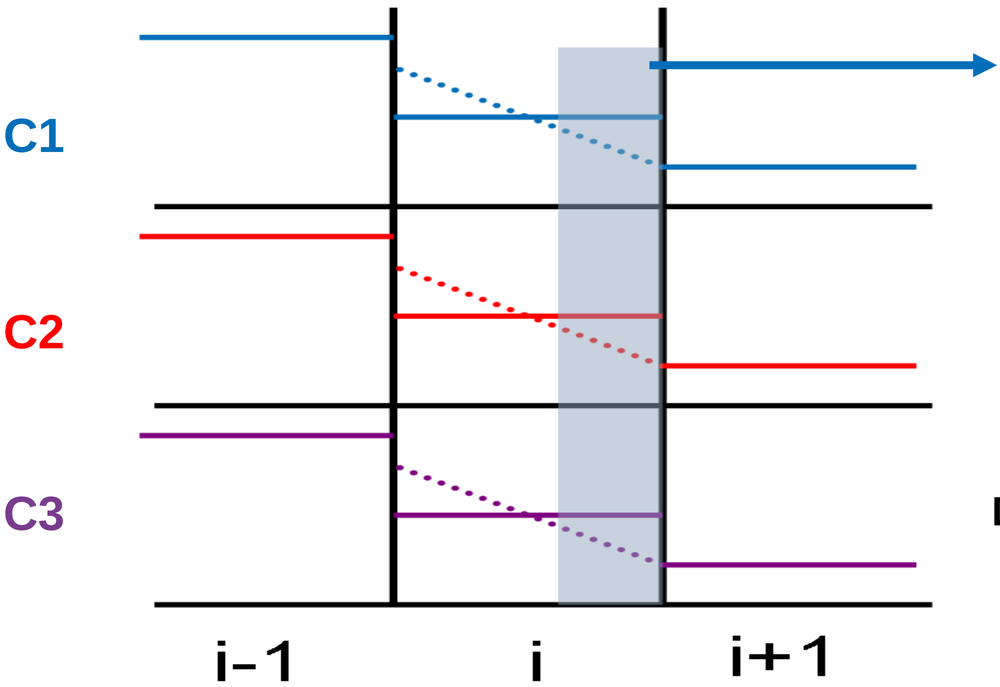


Feasability condition (3/3)

- $c_k = \dfrac{m_k}{m_0}, \; k = 1..3$ $\Rightarrow$ $\partial_t c_k + u \partial_x c_k = 0$
- Reconstruction



Feasability condition not satisfied

$$(1, c_1, c_2, c_3)^t$$

Not a moment vector

$\Rightarrow$ **Canonical moments** *(Dette & Studden 97)*

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Advection: conclusion

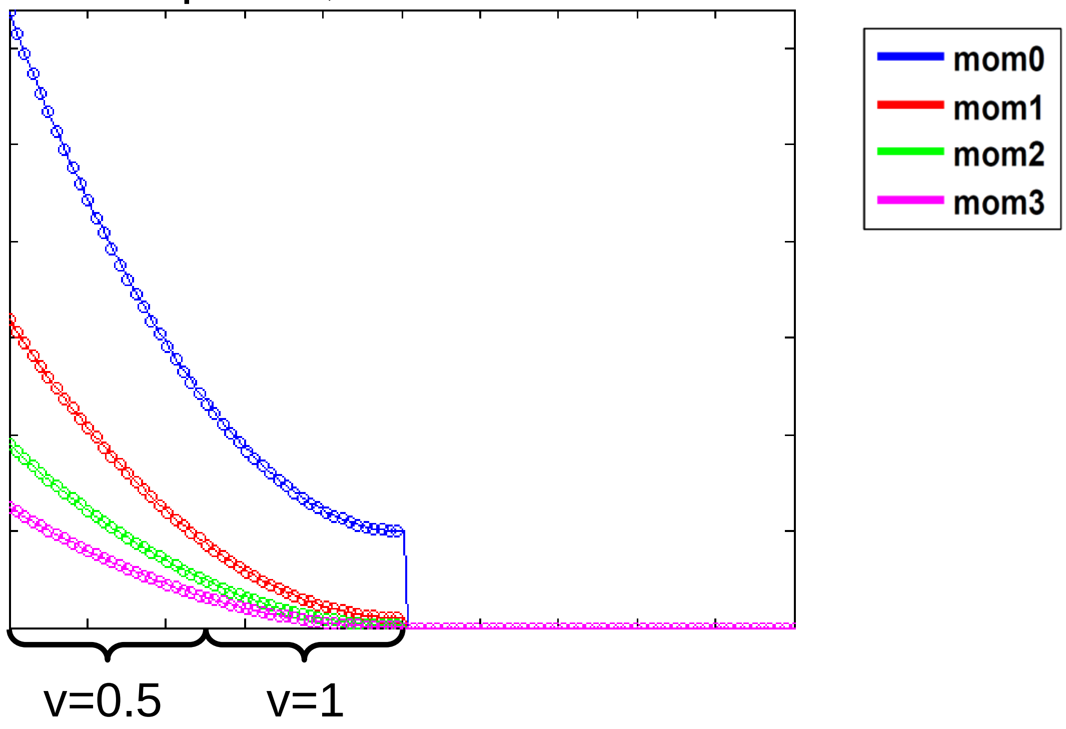
- 2nd order scheme for advection of a moment set
  - Kinetic scheme
  - Canonical moment theory *(Dette & Studden 97)*
- Application:

- Implementation of these tools in IFP-C3D

- Application in other domains:
  - Combustion
  - Meteorology: (*Wright07, McGraw07*)

Advection-Evaporation: Results (1/2)

- $\partial_t f + \partial_x (v f) + \partial_S (R f) = 0$
- N=200 points, 4 size moments



Advection-Evaporation: Results (1/2)

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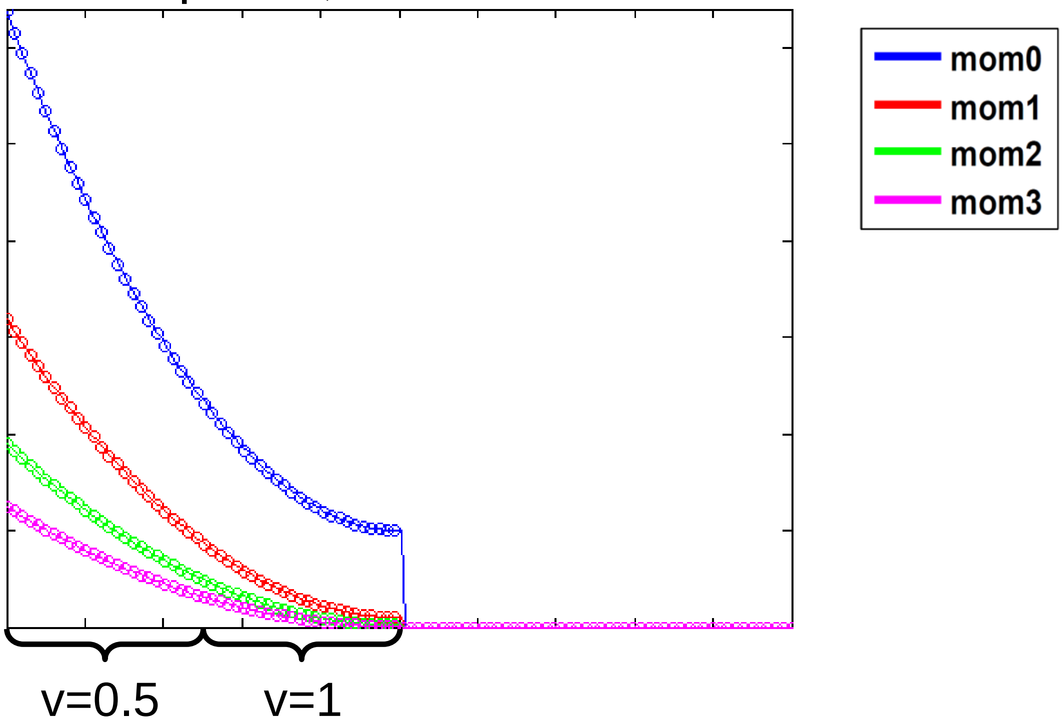
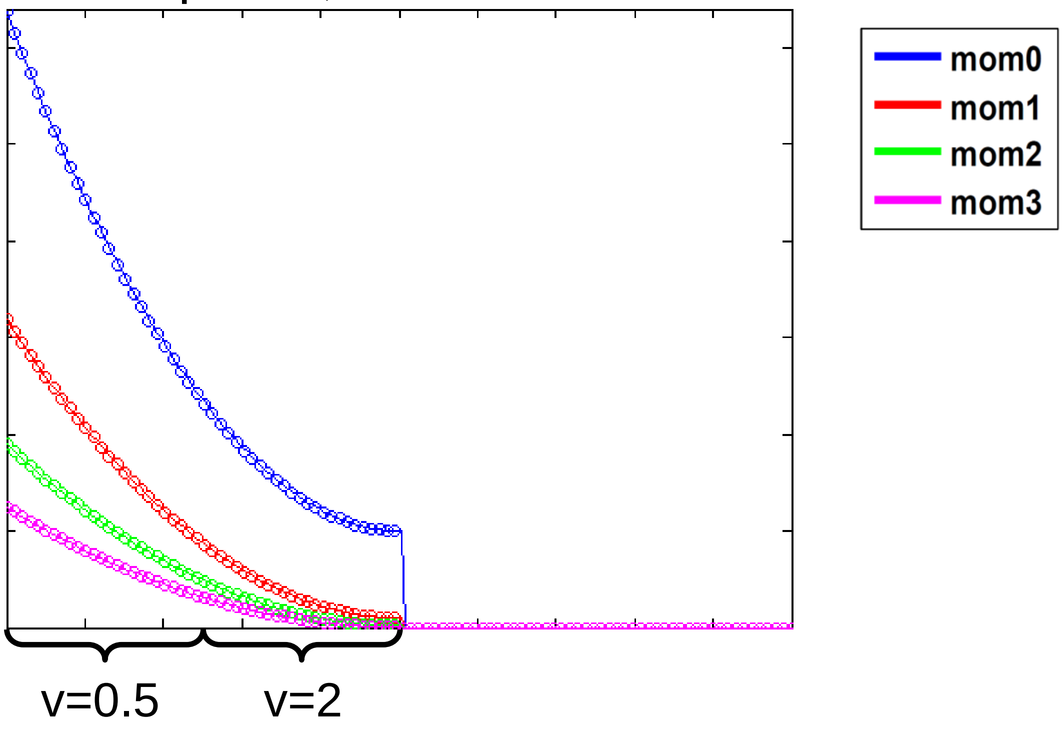


▪Transport of the moments

▪Vacuum zone handled

Advection-Evaporation: Results (2/2)

- $$\partial_t f + \partial_x(vf) + \partial_S(Rf) = 0$$
- N=200 points, 4 size moments



•Dilute flow

•No collision

Advection-Evaporation: Results (2/2)

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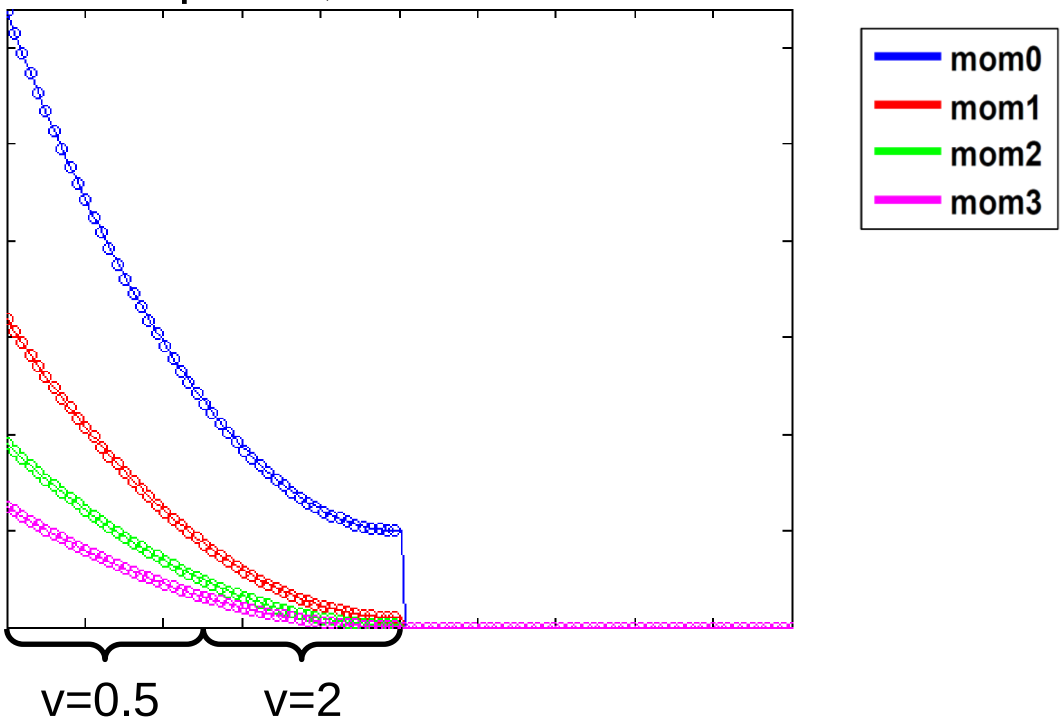

•Dilute flow

•No collision

- Singularity handled
- Not physical

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Conclusions

- **Objectives**

  Design a model and numerical schemes for **advection** of size **moments** of an **evaporative polydisperse** spray, in a **two-fluid** formalism:

- **Achivements:**
  - High size moment model and numerical scheme for evaporation
    - M.Massot, F.Laurent, D.Kah, S. de Chaisemartin: A robust moment method for evalution of the disappearance rate of evaporating sprays, submitted to SIAM journal of applied mathematics available in HAL (2008)
  - High size moment model and 2nd order numerical scheme for advection
    - D.Kah, F. Laurent, M. Massot, S. Jay: A high order moment method simulating evaporation and advection of a polydisperse liquid spray, to be submitted to Journal of Aerosol Science (2009)
  - Theoretical and numerical problems solved
  - Methods applicable in other fields (soots, meteorology)

Perspectives

- Implementation of these tools in the code IFP-C3D to simulate the dispersed phase
- Test cases in 2D and 3D
- Coupling with the separate phase
- High order velocity moments to overcome singularities *(Fox 08)*
    - S. De Chaisemartin, L . Fréret, D. Kah, F. Laurent, R.O. Fox, J. Réveillon, M. Massot: Turbulent combustion of polydisperse evaporating sprays with droplet crossing: Eulerian modeling and validation in the infinite Knudsen limit, proceedings of CTR (2008)

Thank you for your attention

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