

CPU Efficient Modelling of Biomass Gasification Using a Stochastic Reactor Approach and Chemistry Guided Reduction

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Introduction

This paper presents a stochastic reactor model (SRM) for biomass pyrolysis using detailed chemistry and reduced chemistry. The work is divided into two parts:

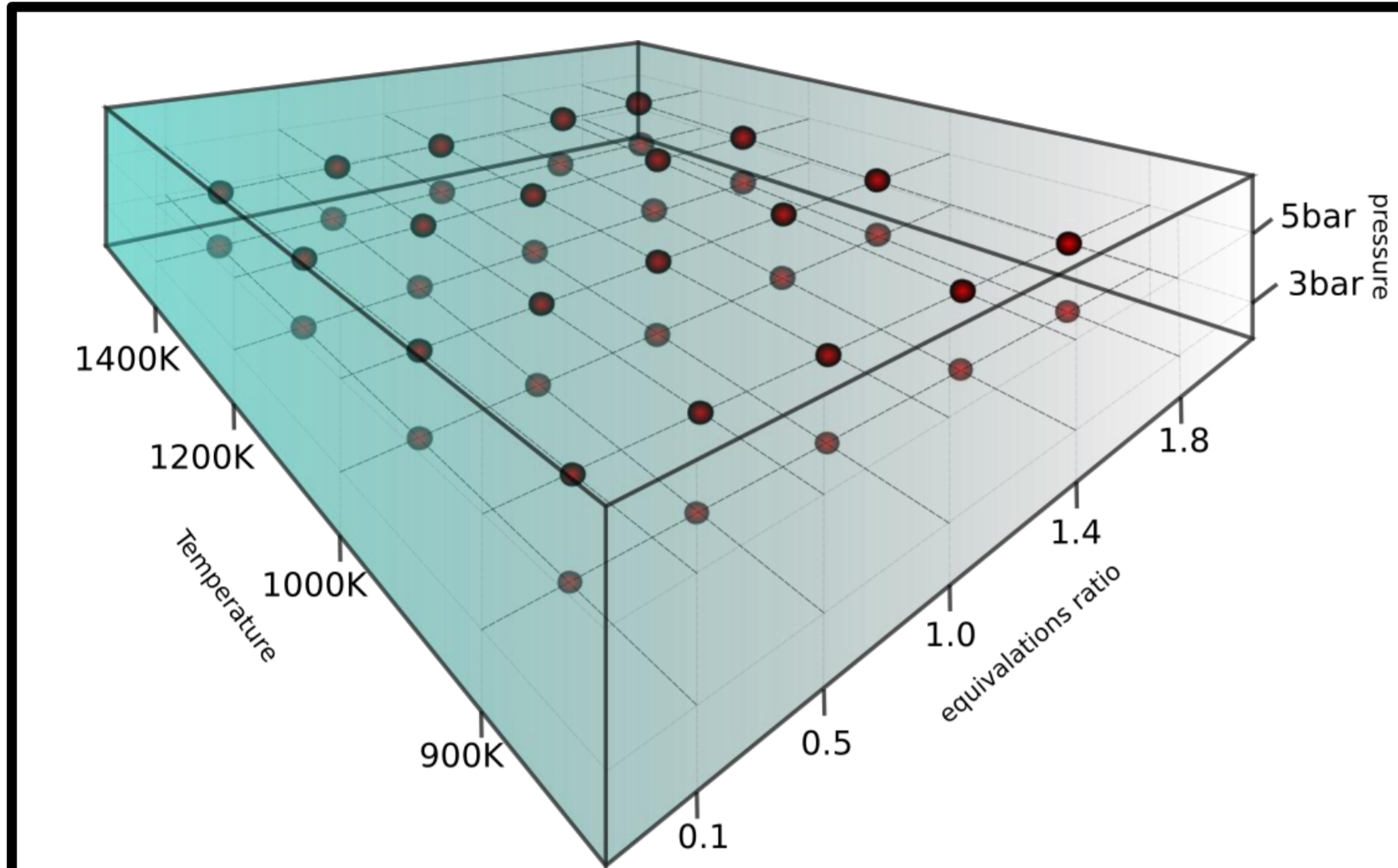
- Development of the multiphase reactor model
- Reduction of a detailed biomass scheme to skeletal size

The developed gasification model is integrated in the software suite LOGEsoft and features a user friendly GUI. For the investigations in this work we used the two following reaction schemes:

- Solid devolatilization kinetics: M. Calonaci et al. 2010 [1]
- Gas phase chemistry: Ranzi et al. 2008 [2] (Biomass scheme from the CRECK Group 12-2012)

The model is compared to the data published by Dupont et al. 2009 [3]

Automatic Reduction of Gas Phase Chemistry



Visualization of a matrix input of target points for ignition delay

- Representative gas mixtures are obtained by running gasification simulations with devolatilization kinetics only
- Reduction of the gas phase chemistry in constant pressure reactors using chemistry guided reduction [3]:
 - Carry out a necessity analysis (optionally with sensitivity analysis) and remove the least necessary species over all reactors
 - Comparison of reduced mechanism to the detailed scheme
- Application of the reduced gas phase chemistry in the gasifier simulation.

Results

The model is compared against the experiments from Dupont et al. (2009):

- Softwood mixture with 0.4 mm
- Reactor length: 1.0 m
- Temperature: 1073 K
- Composition of biomass based on the given analysis in the publication

Mechanism Reduction:

- Detailed gas phase mechanism consists of 327 species and more than 10 000 reactions
- Reduced gas phase mechanism about 60 species and 150 reactions
- The solid phase mechanism with 17 species and 24 reaction was not reduced

Species	Experiment (Dupont 2009) [m%]	Model prediction Detailed scheme [m%]	Model prediction Reduced scheme [m%]
H ₂	1.2	2.5	2.3
CO	43.0	52.8	49.2
CO ₂	7.0	9.7	10.3
CH ₄	4.4	7.7	8.1
C ₂ H ₄	5.0	5.3	6.4
C ₂ H ₂	1.1	1.5	1.3
C ₂ H ₆	No. meas.	0.4	0.5
H ₂ O	11.0	8.7	8.8

The table below shows the total CPU time on and the speedup due to reduction.

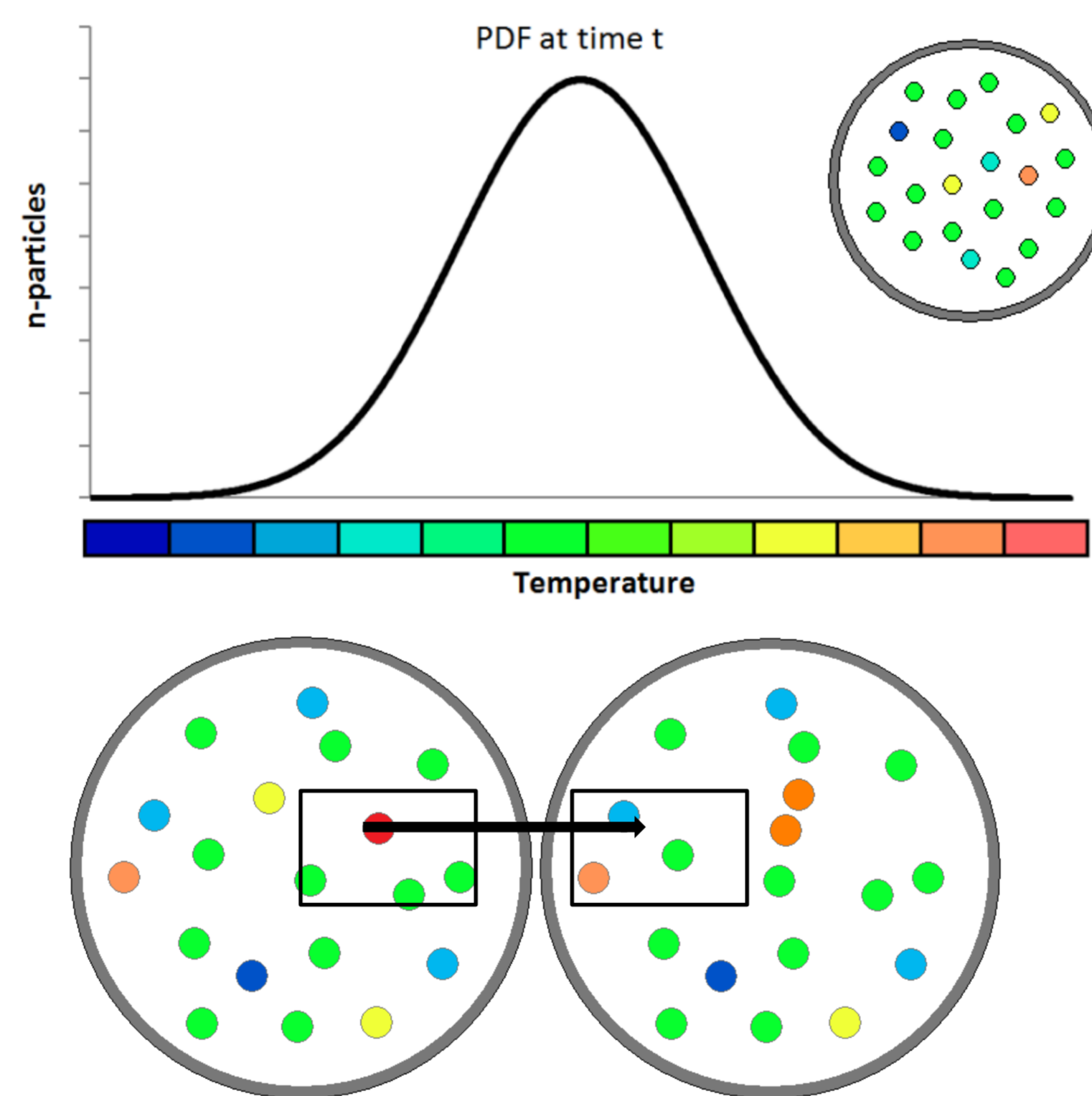
Number of Species	CPU time [s]	Speed up in comparison to 372 species
327	21304	1.0
132	2674	8.0
72	861	24.5
65	857	25.0
64	833	26.0

Since the code is full parallelized the real calculation times are ~10min on a 8 core workstation.

Stochastic Reactor Model

Stochastic Reactor Models is based on probability density functions (PDF):

- Relevant variables are distributed over a number of virtual particles
 - models capture in-homogeneities in the gas / surface
 - particles mix with each other and exchange properties
- Mixing is used to simulate turbulence
 - A stochastically controlled mixing time is employed
- Particles are randomly selected to exchange heat with the reactor walls
 - Heat transfer occurs at intervals dictated by an exponentially distributed waiting time
 - User parameter determines ratio of particles participating in heat transfer



Reactor is discretised into a number of cells:

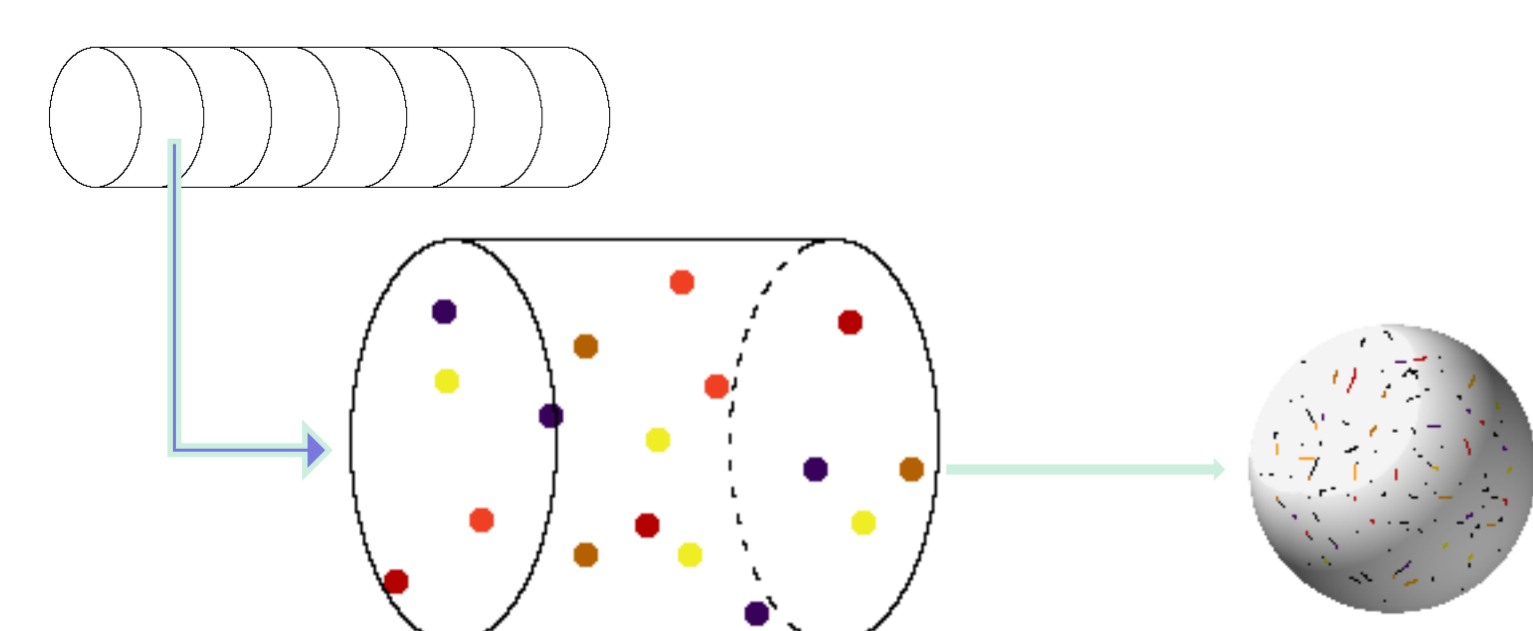
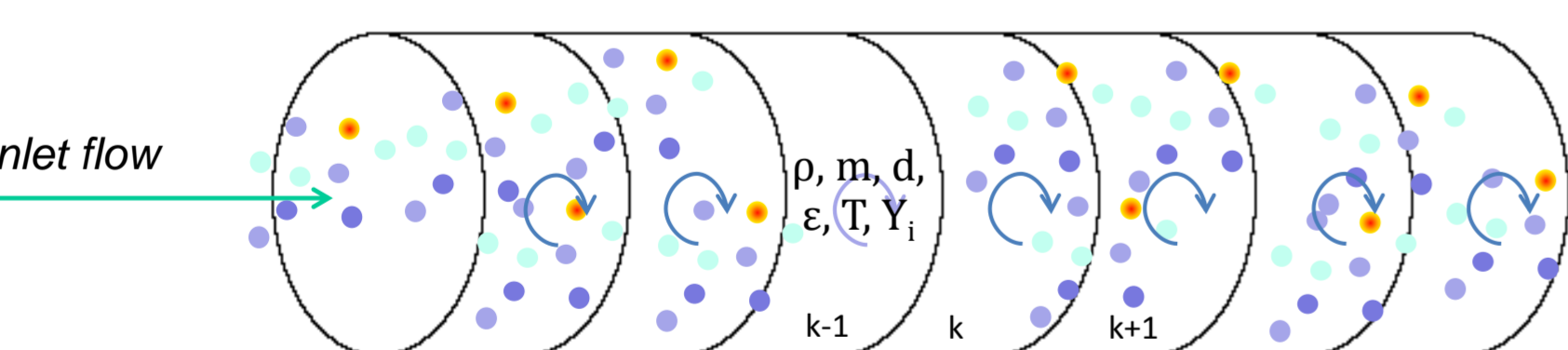
- Each cell is a stochastic, constant pressure, partially stirred reactor
- Flow and chemistry are decoupled with chemistry variables updated at cell centres and flow variables at cell borders

Gas in each cell is distributed over a number of virtual gas particles:

- Each gas particle contains 0–*n* solid particle ensembles
- Gas and solid materials are treated as though moving together
- The effect of recirculation zones is assumed to be negligible

The following phenomena are handled:

- Drying
- Devolatilisation of biomass
- Gas phase reactions
- Cracking
- Char gasification
- Soot formation



- There is no direct interaction between particle types
- Mixing is phase specific
- Solid and pore mass and solid phase physical properties such as porosity and diameter are not mixed
- All solid matter in a gas phase particle is modelled by a single solid particle.

Conclusions

The outcome of this work can be summarized as following:

- ✓ A fast stochastic reactor model for gasification was developed.
- ✓ This tool is capable to use mechanism in standard format and features an intuitive GUI.
- ✓ The model was successful evaluated against experimental values using published reaction schemes.
- ✓ The gas phase chemistry was successful reduced by factor 5 and a speed up of factor of factor 26 was reached.
- ✓ The detailed and the reduced scheme show a good agreement with experimental values for different wood types and sizes.

References:

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