COMPUTATIONAL MODELING OF MIXING AND HEAT TRANSFER IN LAB-SCALE CIRCULATING FLUIDIZED BEDS FOR BIOMASS GASEIFICATION

Jefferson L. M. A. Gomes, j.gomes@imperial.ac.uk
Christopher C. Pain, c.pain@imperial.ac.uk
Imperial College London, Earth Science and Engineering Department, Applied Modeling and Computational Group, London, SW7 2AZ, UK

Jian Su, sujian@con.ufrj.br
Universidade Federal do Rio de Janeiro, COPPE, Nuclear Engineering Program, CP 68509, Rio de Janeiro, 21941-972, Brazil

Abstract. *The optimization of circulating fluidized beds (CFB) operations, in particular their chemical conversions and geometric configurations, have been extensively investigated by a number of researchers. Such studies involve: chemical kinetics in gas-solid reactor models (from packed beds to fast CFB's), numerical investigation of complex geometries, heat transfer models and detailed modeling of biomass gaseification. For these complex models, the Two-Fluid Granular Temperature Model (TFGTM) has been used as it has the flexibility to deal with complex geometry and large number of particles. In this work, computational simulations of 3-D lab-scale CFB were performed to numerically investigate the heat transfer behavior from externals to uniform spherical particles through the TFGTM. The outflow thermal properties (density, velocity, temperature and diffusivity) of the fluid phase may be used to help optimizing the whole circuit plant in a future work.*
Keywords: *CFD, Multiphase Flow, Fluidization, Biomass Gaseification, CFB*

1. INTRODUCTION

Fluidization technologies are used in a wide range of chemical, biochemical, nuclear and energy generation processes with a budget of a trillion dollars annum (Kunii & Levenspiel, 1991). In particular, gas-solid fluidized beds play an important role in several industrial applications due to their high operational efficiency in chemical conversion, heat and mass transfers and particle mixing.

The optimization of circulating fluidized beds (CFB) operations, in particular their chemical conversions and geometric configurations, have been extensively investigated by a number of researchers (Kehlenbeck *et al.*, 2001). For instance: Levenspiel (2002) reported the chemical kinetics in gas-solid reactor models, from packed beds to fast CFBs; Harris *et al.* (2003) investigated the influence of the exit geometry of CFBs on pressure fluctuations; Kehlenbeck *et al.* (2001) experimentally studied the behavior of a CFB used in the pilot plant for the gasification of biomass, and proposed some expressions to correlate particle properties and the CFB performance. In this work, the methods used to solve the two-fluids granular temperature equations are presented and applied for demonstration purposes to the modeling of 3-D circulating fluidized beds.

Although the transport terms in the governing equations are often very simple, their numerical solution is plagued by difficulties associated with simultaneously achieving accuracy and physical realism. This aim is achieved in part with the development of the high resolution finite element method (HRFEM) which provides the spatial accuracy of the discretized transport terms. This is similar to the control volume finite element method (CVFEM) (see Baliga & Patakar, 1983) with the difference being the use of a consistent mapping between the control volume (CV) and the finite element method (FEM) solutions. Since the HRFEM method can result in down wind coupling it is not suitable for discretizing the time domain in time dependent problems. The authors presented elsewhere (Pain *et al.*, 2007, 2005, 2001) a two-level time stepping method that does not have 'backwards coupling' but still achieves, globally, second order accuracy in time and preserves monotonicity with the use of a temporal limiter.

The set of equations associated with the multiphase flow, applied to this problem, involve the solution of a large set of transport equations for density, volume fraction, phase energy and various other fields. The granular temperature model is used to represent the particle-particle interactions which is based on an analogy between particle motion and the motion of gas molecules as described by Lun *et al.* (1984) and Jenkins & Savage (1983).

This work reports the first part of the modeling and optimization of the whole biomass gaseification circuit. In particular, this work shows the robustness of the numerical methods that are used to model the hydrodynamics and heat transfer in dilute flows in a simple 3-D geometry. The TFGTM and the solution method are briefly described on Section 2. The lab-scale riser geometry, thermophysical properties and boundary and initial conditions are described on Section 3. 1, followed by numerical results.

2. THE TWO-FLUID GRANULAR TEMPERATURE MODEL

The gas-solid motion in CFBs is modeled through the the two-fluid granular temperature approach, in which both phases are continuous and fully interpenetrating. These phases are described by separated conservation equations with interaction terms representing the coupling between the phases. The rheology of the granular phase is a function of the solid viscosity and the normal stress, which are obtained from empirical correlations. Therefore, in order to obtain a consistent model which does not rely on purely empirical correlations, Jenkins & Savage (1983) and Ding & Gidaspow (1990) derived these terms using an analogy between the particle-collision during granular flows and the gas kinetic theory. The granular temperature, i.e., the mean deviatoric velocity of a lattice of elastic particles, provides the link between kinetic theory and traditional fluid mechanics.

In the TFGTM framework, mass, momentum and thermal energy balances are described for each phase, and as the average fields of one phase are dependent on the other phase, interaction terms naturally appear in the balance equations, representing the momentum and thermal energy transferred between the phases (Table 1). The full description of these balance equations can be found in Gomes *et al.* (2007a) (see also Gomes *et al.*, 2007b, 2004; Pain *et al.*, 2005). The TFGTM require additional closure laws to describe the rheology of the particulate phase. These closure laws are based on the assumptions of kinetic theory for dry granular flows and are fully described by Gomes *et al.* (2007a) (see also Gomes *et al.*, 2003, 2004; Huilin *et al.*, 2003).

A high resolution method is used to solve the continuity and fluctuation energy equations, and the momentum equations are solved using a non-linear Petrov-Gale rkin method. A time-discretization method based on Crank-Nicolson time stepping is used to ensure time accuracy (see Pain *et al.*, 2001, 2005, for further details.).

The numerical simulation was performed in cartesian geometry. Quadrilateral elements provided a bi-linear variation of velocity and piece-wise-constant variations of volume fraction, pressure and granular temperature. A high resolution method is used in this work to achieve bounded physical meaningful solutions that are also highly accurate. The method used to limit the spatial derivatives is based on the NVD approach (Leonard, 1991) in which face variables are calculated from the element centred values of the field being solved. The variation of these face variables over each face is then limited using the NVD approach so that, if a local extrema is found, then the method switches to a first order spatial discretization. This switching is performed in a smooth manner and depends on a extrema-detecting variable.

A second order temporarily limited time stepping method (based on the Crank Nicolson method) is used in this work to achieve bounded solutions, e. g., positive volume fraction. In order to maintain consistency with the discretized continuity equation, pressure as well as volume fractions have a piecewise constant variation across each hexahedral element. For similar reasons the granular temperature equations are also discretized using the high resolution method described above. The velocities have a tri-linear variation across each element and are thus centred on the nodes of the finite element mesh. The momentum equations are discretized using a Bubnov-Petrov-Galerkin method by multiplying each of the momentum equations for the three velocity components by finite element basis functions and integrating the resulting pressure term by parts. A non-linear Petrov-Galerkin method is used to suppress velocity oscillations normal to the flow direction. The momentum equations are discretized in time using implicit Crank-Nicolson time stepping (Pain *et al.*, 2007).

A semi-implicit projection method is used to solve the coupled multiphase continuity and momentum equations. This method treats the coupling between the phases implicitly in pressure. A mixed finite element method with a constant variation of pressure throughout each element and a bi-linear variation of velocity is used here to avoid singularities in the discretized equations (Pain *et al.*, 2001; Gomes *et al.*, 2007b).

3. TRANSPORT METHODS APPLIED TO GRANULAR DILUTE FLOW PROBLEM

3.1 Description of the Numerical Experiments

In this work, numerical simulations were performed in a 3-D riser. Spherical particles with diameters of 500 μm ($\rho_s = 2660$ kg.m^{-3}) along with air were fed into the domain at a constant throughflow rate and inlet gas velocity. After the initial loading of particles, a quasi steady-state is reached from which the analysis described here was performed. Initial conditions and general configurations used in the simulations are described in Table 2. A riser of diameter 7.62 cm and of height 100.0 cm (Fig. 1) is loaded with particles at a throughflow rate of 40.0 kg.m^{-2}.s^{-1}. The inlet superficial gas velocity was 4.0 m.s^{-1} (a full description of the numerical experiment may be found in Gomes *et al.*, 2003). All the simulations were initialized with a uniform solid volume fraction of 0.03.

As a boundary condition, zero shear stress conditions were applied to the solid phase at the top of the domain. Wall boundary conditions for the particulate phase as described by Jenkins & Savage (1983) were used in these simulations. Air, at standard temperature and pressure, was modeled as a compressible Newtonian fluid, assuming ideal gas behavior. In addition, both the fluid and solid phases, are free to leave the domain through the top boundary. A Dirichlet boundary condition is imposed in the walls for the temperature field. The numerical simulation was performed over 168 seconds.

Table 1. Conservation equations.

Continuity equation	$\frac{\partial}{\partial t}\left(\varepsilon_k \rho_k\right) + \frac{\partial}{\partial x_i}\left(\varepsilon_k \rho_k v_{ki}\right) = 0$
Momentum equation	$\frac{\partial}{\partial t}\left(\varepsilon_k \rho_k v_{ki}\right) + \frac{\partial}{\partial x_j}\left(\varepsilon_k \rho_k v_{ki} v_{kj}\right) = -\varepsilon_k \frac{\partial p_g}{\partial x_i} + \varepsilon_k \rho_k g_i + \beta\left(v_{k'i} - v_{ki}\right) - \frac{\partial}{\partial x_i}\left(\tau_{kij}\right) - \Gamma_k v_{ki}$
Thermal energy equations	$C_{p_g} \rho_g \epsilon_g \frac{DT_g}{Dt} = -p_g\left(\frac{\partial}{\partial x_i}\varepsilon_g v_{g_i} + \frac{\partial}{\partial x_i}\varepsilon_s v_{s_i}\right) + \frac{\partial}{\partial x_i}\left(\varepsilon_g \kappa_g \frac{\partial T_g}{\partial x_i}\right) + \alpha\left(T_s - T_g\right) + \widehat{\Gamma}_{wg}$ $C_{p_s} \rho_s \epsilon_s \frac{DT_s}{Dt} = \frac{\partial}{\partial x_i}\left(\varepsilon_s \kappa_s \frac{\partial T_s}{\partial x_i}\right) + \alpha\left(T_g - T_s\right) + \widehat{\Gamma}_{ws} + S_f$
Granular energy equation	$\frac{3}{2}\left[\frac{\partial\left(\varepsilon_s \rho_s \Theta\right)}{\partial t} + \frac{\partial}{\partial x_j}\left(\varepsilon_s \rho_s v_{s_j} \Theta\right)\right] = \tau_{s_{ij}} \frac{\partial v_{s_i}}{\partial x_j} - \frac{\partial q_j}{\partial x_j} - \gamma - 3\beta\Theta$

3.2 Investigation of Cluster Motion in 3-D Cylindrical Risers

After the initial particle loading, when the riser contents become denser, a quasi steady-state regime is reached and a quasi-periodic behavior is established. Particles move upwards and can either leave the domain, or fall in the near wall region. As they fall, they may collide with rising particles and form particle clusters which vigorously move upwards and downwards. As the clusters fall and crash against the bottom region, the particle clusters break up and splash onto the opposite wall, passing through the center line of the riser and promoting strong recirculation and mixing (see Gomes *et al.*, 2004).

The time-averaged granular temperature calculated from the simulation at the wall and central regions demonstrated a rising in the kinetic energy dissipation in the near wall region. As the core region has a lower particle concentration, the time-averaged granular temperature is lower than in the wall region. However, in the upper regions, i.e., at the exit zone, large granular temperatures may occur in the core region. In addition, the bouncing of particles at the exit zone may lead to either particles falling back into the domain or leaving it unhindered. The overall results obtained from this simulation qualitatively agree with the granular flow behavior reported by Huilin *et al.* (2003), in which a core-annular structure characterizes the flow, i.e., in a time-averaged sense, particles are concentrated in the wall region, whereas in the core, larger velocities promote fast particle transport.

Gomes *et al.* (2004) described the cluster structures as 'vertically elongated' similar to a parabola heading downwards, and having a thin tail upwards. In the horizontal cross section, however, the clusters did not show a single shape in the horizontal cross section, varying from a 'quarter arc' shapes which rotate near the wall region, to 'string-like' shapes, in the core region. Such cluster structure may be seen in Fig. 2. The strong mixing in risers improves the heat transferred from the wall to the dilute flow as shown in Fig. 3. The temperature of the fluid phase *versus* the riser height at the wall

Table 2. General systems configurations and initial conditions.

3-D riser diameter (m)	0.0762	3-D riser height (m)	1.00
Inlet gas velocity ($m.s^{-1}$)	4.00	Solid throughflow rate ($kg.m^{-2}.s^{-1}$)	40.00
Initial porosity	0.03	Initial temperature and pressure	20.0^{o}C 1 bar
Particle-particle restitution coefficient	0.97	Particle-wall restitution coefficient	0.90
Friction coefficient	0.14	Wall temperature	100.0 ^{o}C

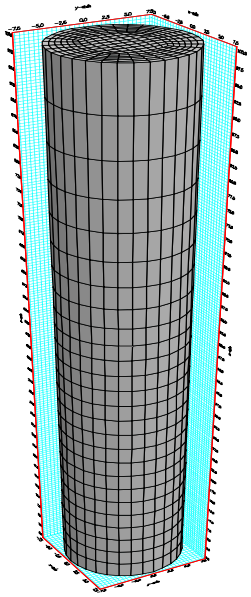


Figure 1. 3-D Riser: schematic with external heater (7371 nodes in 6656 elements).

and center regions is shown in Fig. 4. The temperature in the center region is fairly uniform in the three time-windows shown here, oscillating from 25 to 68^o C. As the clusters randomly bounce in the wall, thermal energy is transferred into the fluid phase and the temperature in the wall region oscillates with a larger amplitude (25-100^o C).

4. CONCLUSIONS

This paper presents a bounded numerical transport scheme that uses an NVD control volume method for the flux limiting and the high-order spatial fluxes are calculated using a finite element method on an unstructured mesh. This is combined with a two level temporally limited time stepping scheme to obtain a monotonicity preserving scheme that has a high degree of global spatial and temporal accuracy. The proposed time stepping method is implicit which may be important for numerical stability reasons where part of the solution domain is discredited with small elements/control volumes. This is especially true of variable resolution and mesh adaptivity applications. Methods like those developed here will become increasingly important with the necessity to combine formal accuracy with physical realism in many transport problems.

In this work, the flow dynamics 3-D risers in operational conditions is modeled by means of the Eulerian-Eulerian CFD code FLUIDITY. The conservative equations, i.e., continuity, momentum, thermal energy (for gas and solid phases) and fluctuation energy (for the granular phase), are solved. Space and time-dependent variables calculated are: solid volume fraction, granular temperature, temperatures, velocities and pressure. The granular kinetic approach used here provides the framework for modeling the dissipation of energy due to non-ideal particle-particle collisions.

Risers are characterized by annular flows in which relatively large particle concentrations $(0.01 \leq \varepsilon_s \leq 0.31)$ move, preferentially, near the wall region while in the core, a dilute particle-flow emulsion is observed. The velocity of particles in the core region are notably larger than those near to the wall. Near the wall, the particles may move upwards or downwards. Such motion may result in clusters of particles crashing into one another and moving towards the opposite wall. The cluster's bouncing helps enhance the heat transfer from externals to the domain promoting a fairly uniform temperature due to the strong mixing. Further work will focus on heat source of chemical reactions from biomass gaseification in complex geometries.

5. ACKNOWLEDGEMENTS

This work is funded by CNPq (55.0359/2005-2, Edital CT-ENERG 17/2005).

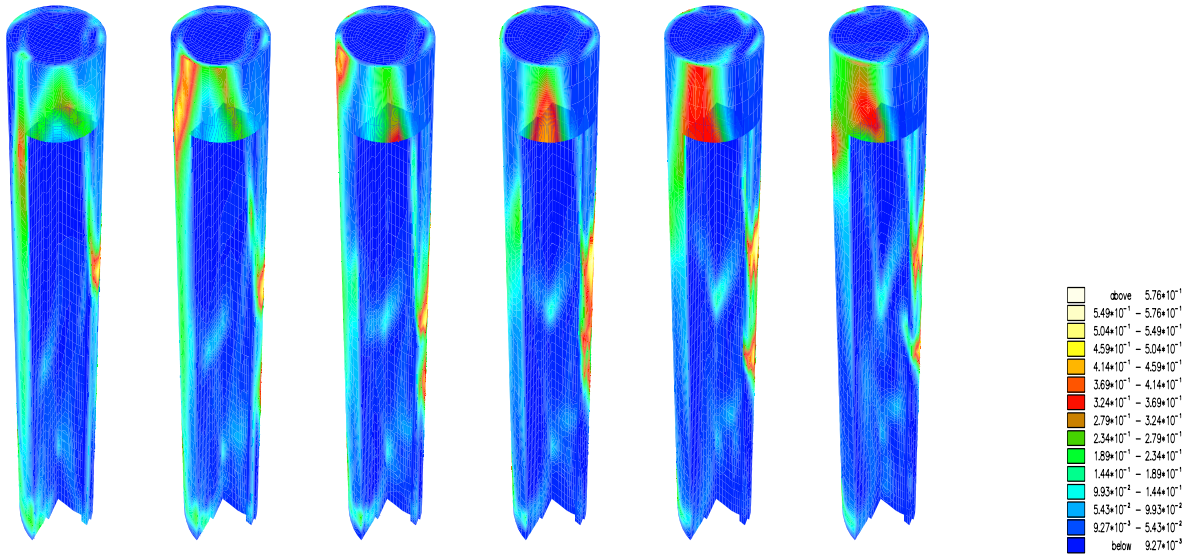


Figure 2. 3-D Riser: Set of frames drawn every 0.04 seconds starting at 3.38 seconds of the numerical simulation. The riser has a diameter of 0.0762 m and a height of 1.0 m, however, only the lower region, i.e., up to 0.3 m is shown. A slice is removed from the domain in order to visualize the cluster motion through the central region.

6. REFERENCES

Baliga, R.B. and Pataker, S.V., 1983, 'A control-volume finite element method for two-dimensional fluid flow and heat transfer', International Journal of Numerical Heat Transfer, Vol. 6, pp. 245-264.

Ding, J. and Gidaspow, D., 1990, 'A bubbling fluidization model using kinetic theory of granular flow', AIChE Journal, Vol. 36, pp. 523-538.

Gomes, J.L.M.A., Pain, C. C., de Oliveira, C.R.E., Goddard, A.J.H., Oliveira, F.B.S., 2003, 'Numerical Investigation of Cluster Formation and Break-Up in Risers Using the TFGTM', Proceedings of the VI Encontro de Modelagem Computacional, Nova Friburgo, Rio de Janeiro, Brazil.

Gomes, J.L.M.A., Pain, C. C., de Oliveira, C.R.E., Goddard, A.J.H., 2002, 'A numerical investigation of the formation and break-up of cluster in 2-D Risers', Proceedings of the IV World Conference in Particle Technology, Sydney, Australia, pp. 230-238.

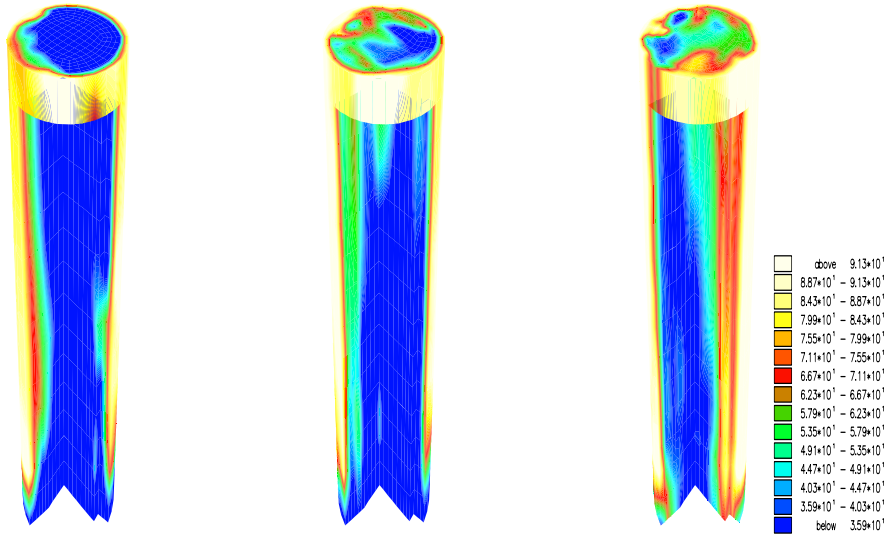
Gomes, J.L.M.A., Pain, C. C., de Oliveira, C.R.E., Goddard, A.J.H., 2007a, 'A Numerical Investigation of Heat Transfer Mechanisms in Gas-Solid Fluidized Beds using the Two-Fluid Granular Temperature Model', Heat Transfer Engineering, Vol. 28, pp. 1-22.

Gomes, J.L.M.A., Pain, C. C., de Oliveira, C.R.E., Goddard, A.J.H., Eaton, M.D., Piggott, M.D., Ziver, A.K., Yamane, Y., 2007b, 'Coupled Neutronics-Fluids Modelling of Criticality within a MOX Powder System - Part II: Transient Analysis', Nuclear Science and Engineering, Submitted.

Harris, A., Davidson, J.F., Thorpe, R.B., 2003, 'Influence of exit geometry in circulating fluidized-bed risers', AIChE Journal, Vol. 49, pp. 52-64.

Huilin, L., Gidaspow, D., Bouillard, J., Wentie, L., 2003, 'Hydrodynamics of binary fluidization in a riser: CFD simulation using two granular temperatures, Chemical Engineering Science, Vol. 58, pp. 3777-3792.

Jenkins, J.T. and Savage, S.B., 1983, 'A theory for the rapid flow of identical, smooth, nearly elastic spherical particles', Journal of Fluid Mechanics, Vol. 130, pp. 187-202.



(a) t = 0.79 s (b) t = 18.63 s (c) t = 27.71 s

Figure 3. 3-D Riser: Snapshots of gas temperature. The riser has a diameter of 0.0762 m and a height of 1.0 m, however, only the lower region, i.e., up to 0.3 m is shown. A slice is removed from the domain in order to visualize the temperature gradient through the central region. Temperature in ^{o}C.

Kehlenbeck, R., Yates, J., Di Felice, R., Hofbauer, H. and Rauch, R., 2001, 'Novel scalling parameter for circulationg fluidized beds', AIChE Journal, Vol. 47, pp. 582-589.

Kunii, D. and Levenspiel, O., 1991, *Fluidization Engineering* (Butterworth-Heinemann Series Editor, London, UK).

Leonard, B.P., 1991, 'The ULTIMATE conservative difference scheme applied to unsteady one-dimensional advection', Computing Methods in Apllied Mechanics and Engineering, Vol. 88, pp. 17-24.

Levenspiel, O., 2002, 'Gas-solid reactor models: packed models, bubbling fluidised beds, turbulent fluidised beds and circulating (fast) fluidised beds', Powder Technology, Vol. 122, pp. 1-9.

Lun, C.K.K., Savage, S.B., Jeffrey, D.J., Chepurniy, N., 1984, 'Kinetic theories for granular flow: Inelastic particles in Couette flow and slightly inelastic particles in a general flow field', International Journal for Multiphase Flow, Vol. 140, pp. 223-256.

Pain, C.C., Mansoorzadeh, S., de Oliveira, C.R.E., Goddard, A.J.H., 2001,'Numerical modelling of gas-solid fluidized beds using the two-fluid approach', International Journal of Numerical Methods in Fluids, Vol. 36, pp. 91-124.

Pain, C.C., Gomes, J.L.M.A., Eaton, M.D., de Oliveira, C.R.E., Goddard, A.J.H., 2005, 'A Model of Heat Transfer Dynamics of Coupled Multiphase-Flow and Neutron-Radiation: Application to a Nuclear Fluidized Bed Reactor', International Journal of Numerical Methods for Heat and Fluid Flow, Vol. 15, pp. 765-807.

Pain, C.C., Gomes, J.L.M.A., Eaton, M.D., de Oliveira, C.R.E., Goddard, A.J.H., 2007, 'Numerical Transport Methods for Multi-Phase Fluid Flow and Radiation Modelling', International Journal of Numerical Methods for Heat and Fluid Flow, Submitted.

7. RESPONSABILITY NOTICE

The authors are the only responsible for the printed material included in this paper.

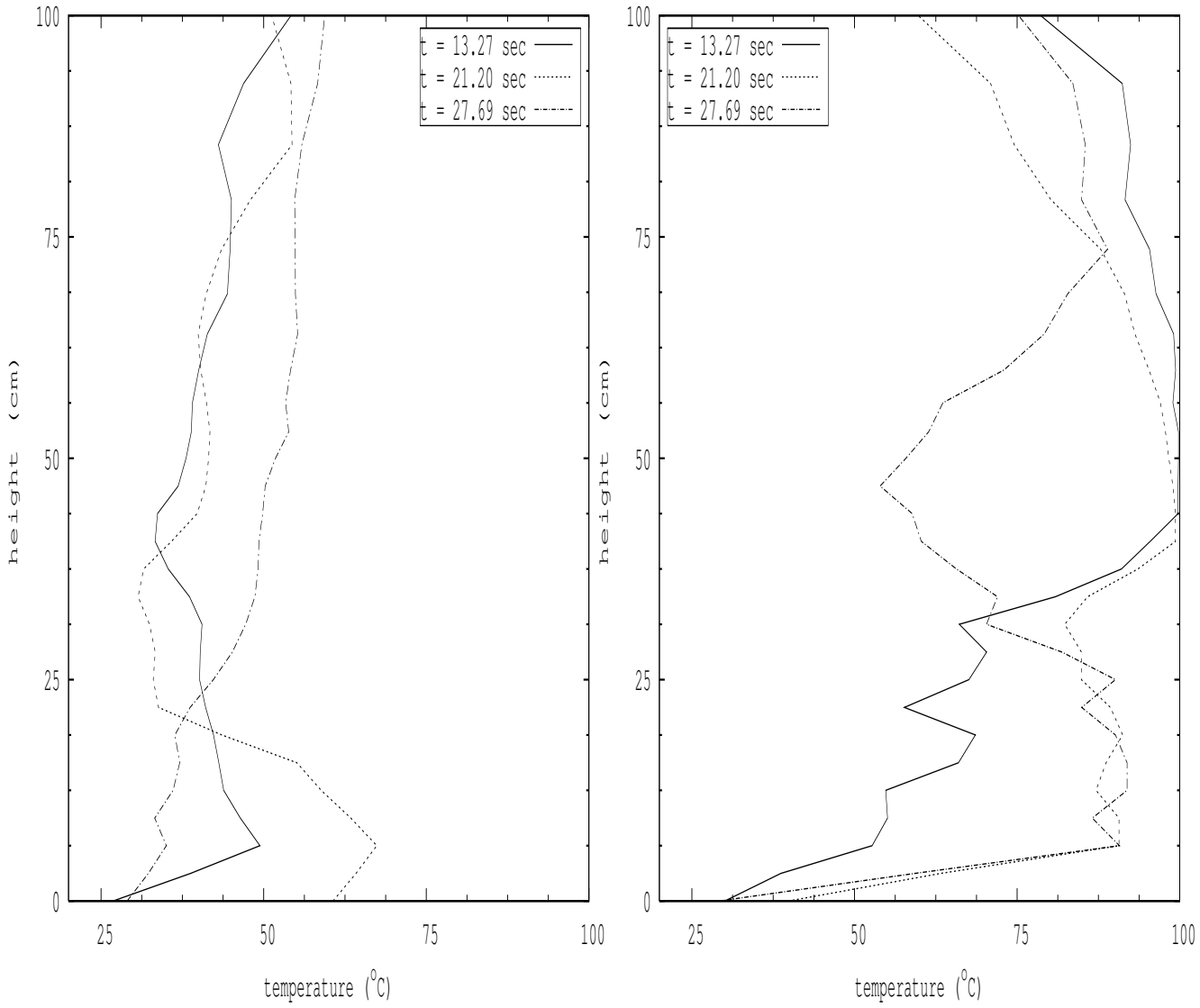


Figure 4. 3-D Riser: Fluid temperature (^oC) *versus* height (cm) of the domain at the (a) center and (b) wall regions at three time-windows.

NOMENCLATURE

C_p	heat capacity (J.(kg.K)$^{-1}$)	T	temperature (K)
g	gravity force (m.s^{-2})	v	velocity (m.s^{-1})
p	pressure (kg.m^{-1}.s^{-2})	x	spatial coordinate (m)
q	flux of fluctuation energy (kg.s^{-3})	r	radial vector (m)
Greek letters			
ε	volume fraction	ρ	density (kg.m^{-3})
$\widehat{\Gamma}$	volumetric wall-phase heat transfer coefficient (W.m^{-3}.K^{-1})	Γ	frictional force exerted on the wall by the phase (N.s.m^{-4})
τ	viscous stress tensor (N.m^{-2})	Θ	granular temperature (m^2.s^{-2})
γ	collisional energy dissipation (kg.m^{-1}.s-3)	β	interphase momentum transfer coefficient (kg.m^{-3}.s^{-1})
α	volumetric interphase heat transfer coefficient (W.m^{-3}.K^{-1})		
Subscripts			
s	solid phase	f	fluid phase
k	phase ($= f, s$)	i , j	coordinates index
w	wall	h	powder component