Forecasting the auto-ignition temperatures of binary liquid mixtures based on BP neural network

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Abstract: The present paper intends to provide a quick effective way for forecasting auto-ignition temperatures (AIT) of the binary flammable liquid mixtures for the chemical engineering projects, the AIT of 168 binary flammable liquid mixtures composed of different components and volume ratios to be chosen as the expected outputs. It has also aimed at selecting the mixed ETSI values of 9 kinds of atom types worked out based on the electro-topological state indices (ETSI) theory as the input variables. It is just for the above said purposes that we have developed a three-layer backward-propagating neural network (BPNN) model for predicting the AIT of binary liquid mixtures according to the atom-type mixed ETSI values and divide the dataset of 168 mixtures randomly into two categories, that is, the training set (140) and the testing set (28). At the same time, we have also selected the gradient descent with the momentum and the adaptive learning rate algorithm as the training function to avoid the slow convergence speed and the low learning accuracy. Thus, we have gained the optimal condition of the neural network by adjusting the various parameters *via* the trial-and-error method, and finding the final optimum structure of BP neural network equal to be 9-8-1. Furthermore, we have also applied the improved Garson algorithm to the multi-parameter sensitivity analysis in assessing the relative and absolute contributions of each atom type through the connection weights of the well trained BPNN model. And, then, we have done the evaluation validation and the stability analysis to validate the model we have proposed, which proves to be obviously superior over the currently existing multiple nonlinear regression (MNR) inductions in terms of the model generalization performance and the prediction accuracy. Along the line, we have identified and determined that the coefficient of the determination (R^2) and the mean absolute error (MAE) of the training set should be equal to 0.965 and 11.892 K, respectively. And, consequently, the coefficient of cross validation (Q^2_{ext}) and MAE of the test set should be equal to 0.923 and 15.530 K, respectively. Moreover, the results of the calculation have shown that the BPNN model enjoys nice fitting ability and forecasting effect, with the predicted error being within the allowable range of AIT experimental error.

Key words: safety engineering; binary liquid mixtures; auto-ignition temperature; BP neural network; prediction

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基于 Pyrosim 的宿舍楼火灾模拟分析*

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摘　要: 为研究不同火灾工况对宿舍楼火灾过程的影响,应用 Pyrosim 对某大学东六宿舍进行火灾动态模拟,对比分析了宿舍大楼所有门窗全开状态和着火房间窗户闭合、门在 20 s 后打开的状态下,宿舍楼各部分温度、烟气层高度、门窗热流量及烟气蔓延特点。Pyrosim 模拟结果表明,在火灾爆发的前 20 s 内,火势发展与门窗开合状态无关。在火灾中后期,门窗全开状态下,着火房间的温度及热流量较低、烟气层离地的高度较高,着火房间上方的宿舍受烟气影响较为严重;而在着火房间窗户闭合、门在 20 s 后打开状态下,横向走廊及各层楼梯处受烟气影响较严重。

关键词: 安全工程;数值模拟;宿舍火灾;Pyrosim 模拟软件;烟气蔓延

中图分类号: X932　　**文献标识码:** A

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0　引　言

学校是人员密集的场所,一旦发生火灾将造成不可估量的损失。而学生宿舍是学校最容易发生火灾险情的地方,因此,学者们对高校宿舍火灾的研究从未停止过,早期的研究主要是通过建立实物模型进行小尺寸的试验研究。但由于其成本高、试验数据缺乏可靠性等不足,限制了人们对宿舍火灾的研究。随着科技的快速发展,计算机仿真技术的出现为海内外学者提供了便利。自 2000 年 2 月美国国家标准与技术研究院(NIST)发布火灾动态模拟软件 FDS(Fire Dynamics Simulator)以来,计算机数值模拟已经成为国内外学者研究各种火灾过程的主要方法[1-4]。Hadjisophocleous 等[5]对一个 10 层的塔楼进行了 FDS 数值模拟并与试验数据进行对比,结果表明,FDS 能够很好地模拟通风良好的高层建筑火灾过程及其烟气运动规律。何明礼等[6]运用 FDS 对腾龙公寓火灾风险进行了研究,探讨了火灾过程中烟气的运动特征和温度的变化情况,结果表明,火灾发展初期烟气快速聚集,温度上升缓慢;当火灾发展到明火燃烧阶段时,室内温度可上升至高达几百摄氏度;安装喷淋系统和排烟系统可以很明显地控制火势的爆发。Glasa 等[7]利用 FDS 建立了电影院火灾模型,结果显示,在给定的火灾场景下,观影厅最危险的地方在于大厅后面和左边部分,并且采用弧形顶棚对观众更加危险。随后,NIST 又在 FDS 的基础上开发了 Thunderhead Engineering Pyrosim,简称 Pyrosim。其最大的特点是提供了三维图形化前处理功能,能方便查看模型,将以前的利用命令行编写建模的 FDS 可视化,使建模更加方便,结果更加直观。梁君海等[8]利用 Pyrosim 模拟了高速列车不同位置着火的火灾场景,得出

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不同位置着火时的危害程度。尚超等[9]运用 Pyrosim 建立了一种适用于 FDS 计算的林木数学模型。由单室的火灾场景模拟[10-11]到大空间高层建筑的火灾模拟[12-14],由隧道交通火灾[15-17]到高空飞机火灾[18-19],计算机数值模拟实现了对全尺寸试验研究不了的方面的探索。

前人模拟的火灾场景多是基于现代建筑,其特点是建筑本身具有比较完善的防火灭火系统,而对于年代久远的建筑防火与逃生尚缺乏理论知识,本文应用火灾动态模拟软件 Pyrosim 对某大学一栋年代久远的东六学生宿舍的两种火灾场景进行动态模拟,研究门窗开合对火灾发展情况的影响,以期为高校宿舍防火灭火及人员逃生提供理论基础,为其他高层建筑(如写字楼、旅馆等)安全防火提供参考。

1 模型建立

1.1 东六宿舍概况

华南理工大学东六宿舍建于 1933 年,由于年代久远,加上当时住宅建设标准低,审批、工程监管、验收以及质量控制整个系统都不健全,宿舍楼的消防系统比较落后,无火灾自动报警系统及喷水灭火系统,只在每层楼道设有两处消防器材放置点。该宿舍楼占地面积约为 1 000 m^2,长 55 m,宽 20 m,每层高 3.2 m 总共 4 层,每层 25 个宿舍,其底层平面图如图 1 所示,每个宿舍长 5.3 m,宽 3.4 m,高 3.2 m,入住 4 人。每个宿舍放置 2 张上下床铺,4 张书桌,2 个衣柜,床铺与书桌分别靠墙两边,无独立卫生间与阳台。宿舍中部及右边设有楼梯,只有一楼中部有 1 个逃生大门。

1.2 火灾场景设置

本文采用 1∶1的比例创建宿舍大楼内部几何空间简化模型,模拟宿舍火灾。图 2 为宿舍楼及着火房间的 3D 效果图,所有墙体表面均为厚 0.013 m 的石膏材料,桌子、柜子和床板表面采用厚度为 0.013 m 的黄松材料,地板表面采用厚度为 0.013 m 的瓷砖材料构成。设计网格边界尺寸略大于宿舍尺寸,为获得最大模拟效率,划分的网格单元数为 2、3、5 的倍数。因此,本文模拟对象网格划分为 110 × 40 × 25,单元格大小为 0.5 × 0.5 × 0.5,单元格总数为 110 000。火源点设置在 2 楼房间 Room 220 床位上铺,火源面积为 0.4 m × 0.5 m,火源功率为 800 kW/m^2,模拟时间为 600 s,燃烧反应物质为聚氨酯。本文的讨论分析均始于火灾产生明火的瞬间,即忽略火灾阴燃阶段。

大楼内部各处设有热电偶探测器,两种火灾工况如表 1 所示,状态 1 的设定对应实际场景为宿舍楼内学生处于活动状态,因此所有门窗皆为打开状态; 状态 2 的设定对应的实际场景为学生处于休息状态,当火灾发生时,位于着火房间的学生在 20 s 内将门打开,逃出房间。两种状态是根据学生在宿舍楼最常见的两种活动而设定,通过模拟这两种状态的火灾场景,可以获得宿舍火灾的发展过程。为获得房间及楼梯温度云图,设置温度切片,其分布如图 3 所示,其中 $x = 8.5$ m 对应着火房间中心平面,$x = 25.0$ m 对应中部楼梯中心平面,$x = 50.5$ m 对应右边楼梯中心平面。

表 1 两种火灾工况描述

Table 1 Description of two kinds of fire scenarios

工况名称	描述
状态 1	所有门窗全开
状态 2	着火房间窗户关闭,门在 20 s 时打开,其他门窗全开

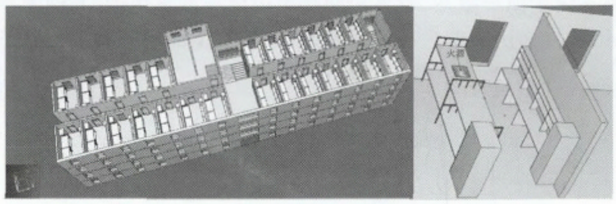

图 2 宿舍楼及着火房间布置 3D 模型图

Fig. 2 3D model of the building and fire room

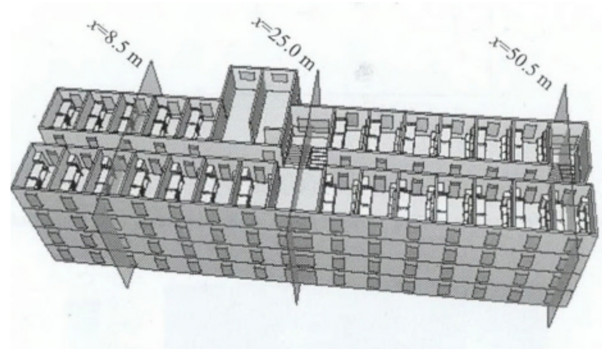

图 3 宿舍大楼切片分布图

Fig. 3 Slice distribution in the building

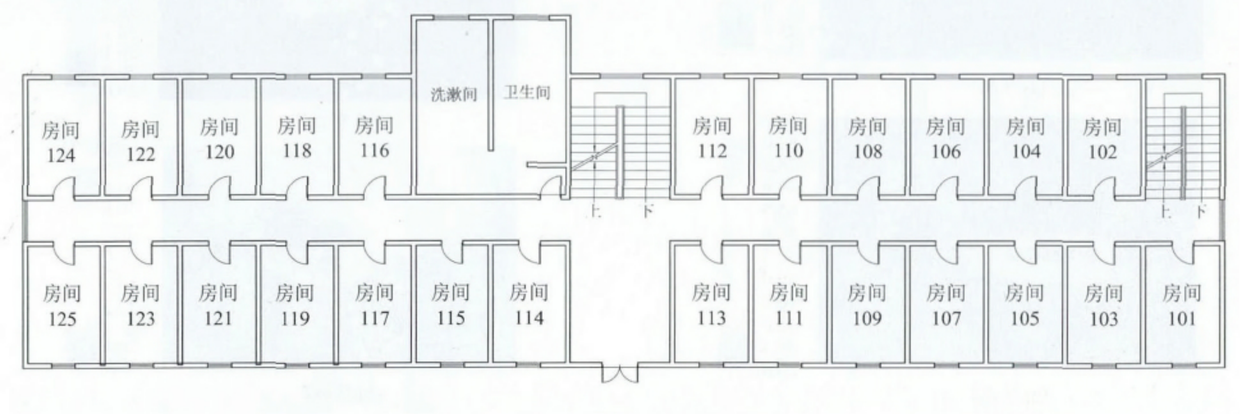

图 1 底层平面分布图

Fig. 1 Layout of the dormitory building

2 模拟结果与分析

2.1 温 度

图 4 为两种状态下着火房间顶棚温度对比图。从图 4 可以看出，着火房间温度均在前 50 s 迅速增加达到最大值，50 s 后缓慢降低逐渐趋于平衡温度。两种状态下的顶棚温度在前 30 s 内是一样的，30 ~ 50 s，状态 2 即着火房间窗户关闭，门在 20 s 时打开状态下温度较高，最高温度和平衡温度均比窗户全开状态高约 10 ℃。在火灾爆发的前 30 s 内，由于热量在短时间内产生，使房间温度升高，但来不及扩散出去，所以着火房间内温度的变化与门窗开合状态无关，但之后，由于窗户敞开，热量会通过窗户传递到外界，从而门窗全开状态下的房间温度会明显低于窗户关闭状态。

图 5 ~ 7 为 $t = 500$ s 时两种状态不同位置温度云图。从图 5 可以看出，状态 1 即门窗全开状态下，着火房间最高温度比状态 2 要小 10 ℃，而着火房间窗户外界与上面房间温度较高。由于窗户敞开，着火房间热量由窗户散发出去，并向上蔓延，从上面房间窗户进入房间内部，使得上面房间温度比状态 2 的温度高。2 楼中部楼梯口处温度分布相差不大，其温度差为 1 ℃，但状态 1 下 3 楼楼梯口温度较高，而状态 2 下楼梯顶部温度较高，见图 6。楼梯离着火房间距离较远的地方，在离火源较远的地方，着火房间门窗开合状态对温度的影响不大。图 7 中，在状态 1 下，右边楼梯各层温度较高区域主要集中在楼梯口处，而状态 2 下，2 楼高温区集中在楼梯口，对于较高楼层，温度较高区域在于楼梯上层空间。窗户关闭的状态下，楼梯处的烟囱效应比窗户敞开状态更为明显。由图 5 ~ 7 可知，状态 2 的温度整体上比状态 1 高，楼梯温度受火灾影响升高的区域也比状态 1 大。从整体上看，着火房间温度较楼梯温度低约 50 ~ 60 ℃，右边楼梯温度相对中部楼梯小。

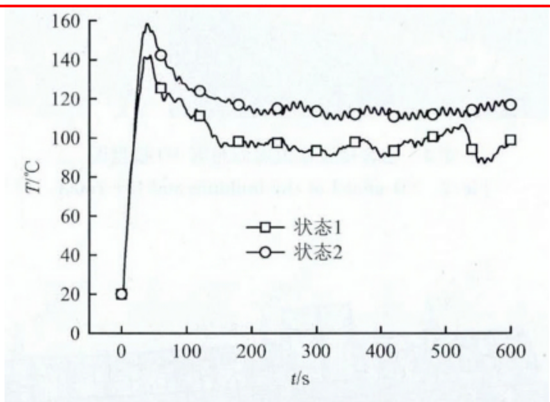

图 4 着火房间顶棚温度对比曲线图

Fig. 4 Fire room ceiling temperature comparison of two conditions

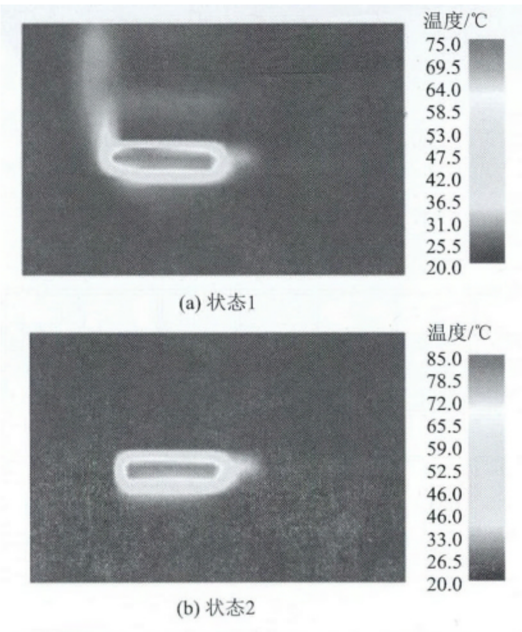

图 5 $t = 500$ s 时 $x = 8.5$ m 两种状态温度云图

Fig. 5 Temperature cloud of two condition at $x = 8.5$ m, $t = 500$ s

2.2 烟气层高度

相对于温度与有害气体，烟气是逃生过程中影响最大的一个方面，研究表明，当烟气层高度低于 2.5 m 时，人员逃生

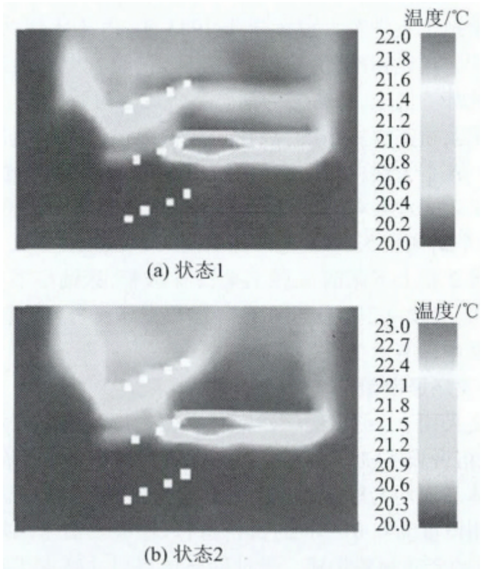

图 6 $t = 500$ s 时 $x = 25.0$ m 两种状态温度云图

Fig. 6 Temperature cloud of two condition at $x = 25.0$ m, $t = 500$ s

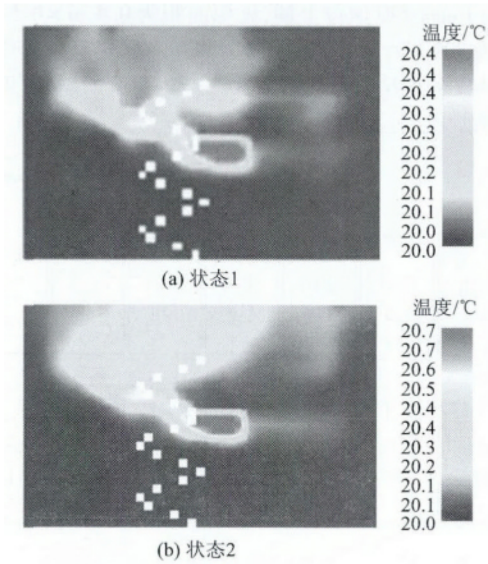

图 7 $t = 500$ s 时 $x = 50.5$ m 两种状态温度云图

Fig. 7 Temperature cloud of two condition at $x = 50.5$ m, $t = 500$ s

将受到严重影响；当烟气层高度低于 1.5 m 时，人员无法完成逃生活动[20]。图 8 为 2 楼着火房间烟气层高度对比曲线图，图中显示，两种状态下烟气层高度变化趋势相同，在 20 s 内迅速下降至最低，然后趋于平衡。因此，位于着火房间的人员须在火灾发生的前 20 s 逃离着火房间，否则，人员生命安全将受到严重威胁。在火灾爆发的前 20 s，两种状态的烟气层高度相同，与门窗开合状态无关，随后状态 1 下烟气层高度下降至 1.4 m，然后保持平衡，而状态 2 下降至 1.2 m，故对于着火房间来说，火灾爆发前 20 s 内，两种状态危险性相同，但在后期，由于在门窗全开状态下，烟气可以通过门和窗户向外扩散，而状态 2 下烟气只能通过门扩散出去，故在 20 s 后门窗全开状态下的火灾形势没有窗户关闭、门在 20 s 时打开状态严重。

2.3　热流量

火灾发生过程中门窗全开，对着火房间的门窗热流量及房间累积热流量进行分析，其结果如图 9 所示。窗户热流量在前 50 s 内迅速增加，最高可达 50 kW，然后逐渐下降至趋于平衡，平衡热流量约为 25 kW，门的热流量在前 25 s 内达到峰值（约 27.5 kW），平衡时的热流量约为 5 kW，房间累积热流量在前 50 s 由最大 160 kW 降至约 90 kW，然后逐渐增大，直至达到最大平衡热流量（约 120 kW）。房间着火时，前 25 s 门与窗的热流量是相同的，25 s 后窗户热流量继续增加，门的热流量则开始减小，在 50 s 时，窗户热流量开始减小，而门的热流量开始趋于平衡，在 150 s 时，窗户热流量开始趋于平衡。火源释放的热功率为 160 kW，房间累积的热流量最低 90 kW，平衡时 120 kW，占总热流量的 1/4。因此，在火灾发生过程中，通过门窗散发出去的热量占少数，大部分热量用于升高着火房间温度。这是因为窗户外为开放的边界，其压力、温度等可以视为恒定不变，虽然外界与走廊的初始条件相同，但走廊为受限空间，当热量传播到走廊时，走廊的温度升高，与着火房间的温度差减少，传热动力减小，因此在 25 s 后，门的热流量会小于窗户的热流量。

两种状态着火房间门的热流量与房间累积热流量对比见图 10。结果显示，两种状态热流量变化趋势相同，在窗户关闭、门在 20 s 时打开状态下，由于热量只能通过门向外扩散，故着火房间门的热流量远高于门窗全开状态，最高热流量为 45 kW，平衡时为 25 kW，均比状态 1 高约 20 kW，见图 10(a)。

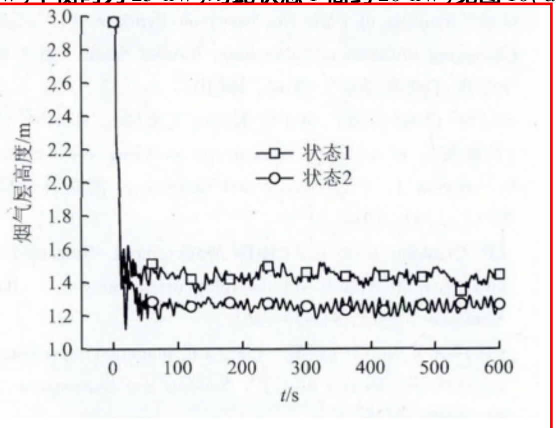

图 8　着火房间烟气层高度对比曲线图

Fig. 8　Comparison of smoke layer height in the fire room

从图 10(b) 可以看出，房间累积热流量最小值要比门窗全开状态高约 25 kW，平衡值高约 15 kW。由此可见，当房间发生火灾时，保持着火房间窗户敞开状态，可适当降低着火房间及走廊热量负荷。

2.4　烟气蔓延

图 11 为 $t = 200$ s 时两种状态烟气蔓延情况，状态 1 即所有门窗全开状态下，走廊及楼梯烟气浓度远没有状态 2 的烟气浓度大，状态 1 下烟气从窗户蔓延出来，导致着火房间上方的房间烟气浓度相对较大，而在状态 2 下，位于着火房间同一层的房间受烟气影响较为严重。图 12 为 $t = 530$ s 时两种状

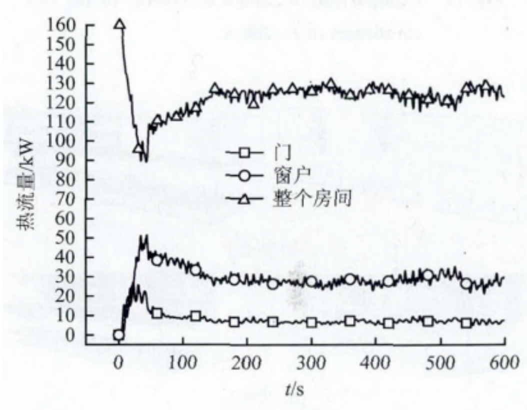

图 9　状态 1 着火房间热流量随时间变化曲线

Fig. 9　Heat flow of fire room with all windows and doors open

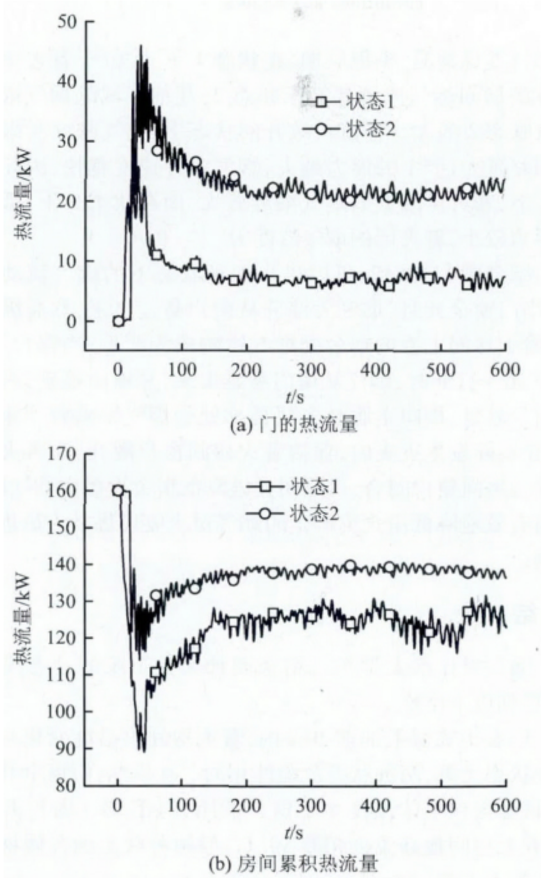

图 10　两种状态着火房间热流量对比曲线

Fig. 10　Comparison of heat flow of two conditions

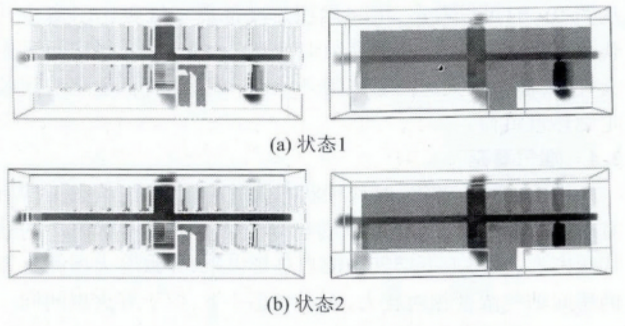

图 11 $t=200$ s 时两种状态烟气蔓延情况对比

Fig. 11 Comparison of smoke movement of the two conditions at $t=200$ s

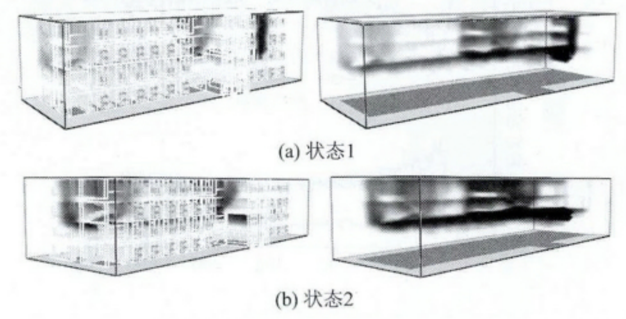

图 12 $t=530$ s 时两种状态烟气蔓延情况对比

Fig. 12 Comparison of smoke movement of the two conditions at $t=530$ s

态烟气蔓延情况，模拟后期，在状态 1 下，除位于着火房间正上方的房间烟气浓度要高于状态 2，其他区域的烟气浓度均没有状态 2 的大。在窗户敞开的状态下，空气密度与烟气密度相差越大，产生的浮力越大，烟气上升速度越快，因此在状态 1 下，着火房间上方烟气浓度较大，而在状态 2 下，烟气上升浮力较小，着火层的烟气浓度大。

结合图 11 和 12，可以得出两种状态下的烟气流动规律为，当门窗全开时，烟气大部分从窗户蔓延出来，然后纵向蔓延，着火房间上方的宿舍受烟气影响较为严重；当窗户闭合、门在 20 s 打开时，烟气从房门蔓延出来，并横向蔓延，再由楼梯向上蔓延，横向走廊及各层楼梯处受烟气影响较严重。因此，在实际发生火灾时，保持着火房间窗户敞开，而着火房间上方的房间窗户闭合，可以明显地降低宿舍大楼内烟气浓度，从而有效地降低由火灾产生的烟气对火灾形势及人员逃生的影响。

3 结 论

通过对比某大学东六宿舍两种火灾工况的动态模拟结果，得到以下结论。

1) 在火灾爆发的前 30 s 内，着火房间内温度变化与门窗开合状态无关，两种状态危险性相同。在后期，门窗全开状态下，宿舍楼内整体温度小于窗户关闭、门在 20 s 时打开状态下，着火房间最高温度相差 10 ℃，但两种状态的各楼梯最高温度相差不超过 1 ℃。

2) 窗户全开状态下，楼梯温度较高区域主要集中在楼梯口处，而窗户关闭、门在 20 s 时打开状态下，楼梯处温度较高区域集中于楼梯上层空间。

3) 在火灾爆发的前 20 s，着火房间内烟气层高度的变化与门窗开合状态无关；20 s 之后，门窗全开状态下的房间烟气层高度比窗户关闭、门在 20 s 时打开状态高约 0.2 m。

4) 通过门窗散发出去的热量仅占 1/4，其余热量用于升高着火房间温度。在 0 ~ 25 s，两种状态门窗以及房间累计热流量均相同；25 s 之后，门窗全开状态下，从窗户散发的热量多于从门散发的热量；窗户关闭、门在 20 s 时打开状态下，门的热流量比门窗全开状态高约 25 kW，房间累积热流量最小值要比门窗全开状态高约 25 kW，平衡值高约 15 kW。

5) 门窗全开状态下，烟气大部分从窗户蔓延出来，然后垂直蔓延，着火房间上方的宿舍受烟气影响较为严重；着火房间窗户闭合、门在 20 s 后打开状态下，烟气从房门蔓延出来，并横向蔓延，再由楼梯向上蔓延，横向走廊及各层楼梯处受烟气影响较严重。

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Analysis of the dormitory building fire risk based on the Pyrosim simulation

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Abstract: This paper is inclined to bring about an analysis of likely-to-be existing factors to cause the dormitory fire risks by taking No. 6 Dormitory of a certain university as a case study sample. In the paper, we have illustrated such factors of the building fire as the temperature, the smoke layer height, the heat flow, and the smoke movement in two different conditions with all the windows and doors being open, or with the windows closed but the doors opened 20 seconds later after the fire broke out. In doing so, we have also set up two conditions according to the two general situations of the students' dormitories (with the students living in at night for sleep and with them engaged in some daily activities). The results of the Pyrosim simulated research indicate that there doesn't seem to have any correlation or correlations between the fire appearance and the two conditions mentioned above during the first 20 s since the fire broke out. And, later, when the doors and windows are opened, high temperature areas of the stairs would come into the room whereas the overall temperature in the dormitory remains lower and the smoke thickness begins to rise abruptly. Comparing the conditions with the windows closed and the door opened 20 s later, the high temperature area of the stairs would become spread over the upper space. Moreover, when the fire broke out, part of the violent heat may tend to propagate through the doors and windows. In such a situation, most of the heat would spread and propagate the high temperature of the fire to the firing room. Furthermore, with the aggravation of the fire disasters, the heat flow from the door and the accumulated heat flow in the firing room may turn to become much lower than that situation with the windows closed and the doors opened 20 s later. Thus, in the whole process, the upper stories of the fire building would be seriously suffered by the smoke in case the windows and doors of the firing room were opened. In contracts, the corridors and stairs would be more seriously affected by the smoke when the room windows in fire are closed with the door opened 20 seconds later.

Key words: safety engineering; numerical simulation; dormitory fire; Pyrosim simulation software; smoke movement

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